

1/7/2005

s 46.150.18/RID (P) 4.214.1/RID  
 13942898 46.150.18/RID  
 13439 4.214.1/RID  
 L4 5762 46.150.18/RID (P) 4.214.1/RID

=> s l4 and ether  
 78010 ETHER  
 933 ETHERS  
 78010 ETHER  
 (ETHER OR ETHERS)

L5 21 L4 AND ETHER

=> d l5 1-21 iall

L5 ANSWER 1 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 719709-67-8 REGISTRY  
 ED Entered STN: 30 Jul 2004  
 CN 7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid, 7-oxabicyclo[4.1.0]hept-  
 3-ylmethyl ester, polymer with  $\alpha$ -hydro- $\omega$ -  
 hydroxypoly[oxy(oxiranyl-1,2-cyclohexanediyl)] ether with  
 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (3:1), and 3,3'-[1,4-  
 phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI) (CA  
 INDEX NAME)  
 MF (C20 H30 O4 . C14 H20 O4 . (C8 H12 O2)n (C8 H12 O2)n (C8 H12 O2)n C6 H14  
 O3)x  
 CI PMS  
 PCT Epoxy resin, Manual component, Polyester, Polyether, Polyether formed,  
 Polyother  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAplus document type: Patent  
 RL.P Roles from patents: PREP (Preparation); USES (Uses)

# Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C20-C6	OC2-C6	3-6	C60	106.32.1	2 in CM 3
C30	OC3	4	C30	4.214.1	2 in CM 2
C6	C6	6	C6	46.150.18	1 in CM 2

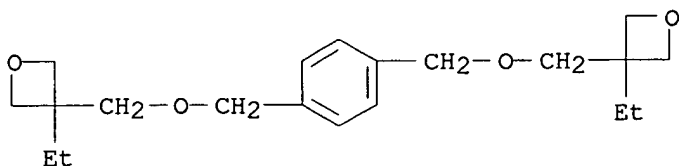
CM 1

CRN 244772-00-7  
 CMF (C8 H12 O2)n (C8 H12 O2)n (C8 H12 O2)n C6 H14 O3  
 CCI IDS, PMS, MAN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

CM 2

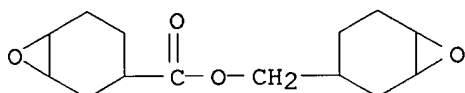
CRN 142627-97-2  
 CMF C20 H30 O4



CM 3

CRN 2386-87-0

CMF C14 H20 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

ACCESSION NUMBER: 141:113883 CA  
TITLE: Light-transmitting epoxy resin sealing material, optical module sealed with the material, and manufacture of the optical module  
INVENTOR(S): Hashimoto, Shinji; Kitamura, Kenji; Nemoto, Tomoaki; Nakashiba, Toru; Yagyu, Hiroyuki; Koderu, Kohei; Ushiyama, Naoki; Matsushita, Tomoaki; Matsushita, Yukio; Kasai, Yuki; Kurai, Hiroyuki  
PATENT ASSIGNEE(S): Matsushita Electric Works, Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
INT. PATENT CLASSIF.:  
MAIN: C08G059-40  
SECONDARY: C08L063-00; C08L071-02; H01L023-29; H01L023-31  
CLASSIFICATION: 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)  
Section cross-reference(s): 38, 76  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004203943	A2	20040722	JP 2002-371881	20021224
PRIORITY APPLN. INFO.:			JP 2002-371881	20021224

#### ABSTRACT:

The material contains an epoxy resin, a crosslinking catalyst, and 0.01-1 mass% (based on the total amount) of  $C_nH_{2n+1}N[(C_2H_4O)_xH](C_2H_4O)_yH$  ( $n = 12-18$ ;  $x + y = 1-10$ ) and/or  $C_nH_{2n+1}C_6H_4O(CH_2CH_2O)_mH$  ( $n = 8, 9$ ;  $m = 2-15$ ). The material is for sealing of a gap between (A) a semiconductor part having the 1st electrode and a light-accepting part and (B) a circuit board having the 2nd electrode, an optical waveguide, and an optical coupler in the optical module, in which the 2 electrodes are connected by a metal bump. The claimed optical module is manufactured by the process involving (a) facing of the light-accepting part and the optical coupler, (b) connecting of the 2 electrodes by a metal bump, and (c)

sealing of the gap between the semiconductor part and the circuit board by the composition. The sealing material contributes to reinforcement of the metal bump and reduction of transmission loss in the optical coupler.

SUPPL. TERM: light transmitting epoxy resin sealant; optical module gap epoxy resin sealant; amine polyoxyalkylene epoxy resin sealant; phenyl ether polyoxyethylene epoxy resin sealant

INDEX TERM: Polymerization catalysts  
(cationic; in light-transmitting epoxy resin sealing material for optical module)

INDEX TERM: Electronic device fabrication  
(for preparation of optical module; light-transmitting epoxy resin sealing material for)

INDEX TERM: Sealing compositions  
Transparent materials  
(light-transmitting epoxy resin sealing material for optical module)

INDEX TERM: Epoxy resins, uses  
ROLE: TEM (Technical or engineered material use); USES (Uses)  
(light-transmitting epoxy resin sealing material for optical module)

INDEX TERM: Optical couplers  
Optical waveguides  
Printed circuit boards  
Semiconductor devices  
(light-transmitting epoxy resin sealing material for optical module having)

INDEX TERM: 1337-30-0, Sorbitan laurate  
ROLE: MOA (Modifier or additive use); USES (Uses)  
(LP 20R; in light-transmitting epoxy resin sealing material for optical module)

INDEX TERM: 56-81-5, Glycerin, uses 63-91-2, Phenylalanine, uses 111-20-6, Sebacic acid, uses 514-10-3, Abietic acid 9016-45-9, Nonion NS 204.5 31017-83-1, Nymeen L 202  
ROLE: MOA (Modifier or additive use); USES (Uses)  
(in light-transmitting epoxy resin sealing material for optical module)

INDEX TERM: 326795-44-2P 719709-67-8P  
ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(light-transmitting epoxy resin sealing material for optical module)

INDEX TERM: 33918-18-2, SA 102 87301-62-0, Adeka Opton CP 66  
ROLE: CAT (Catalyst use); USES (Uses)  
(polymerization catalysts; in light-transmitting epoxy resin sealing material for optical module)

L5 ANSWER 2 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 705284-25-9 REGISTRY

ED Entered STN: 07 Jul 2004

CN 2-Propenoic acid, 2-methyl-, (1-methylethylidene)bis[4,1-phenyleneoxy(2-hydroxy-3,1-propanediyl)] ester, polymer with 1,4-bis[(ethenyloxy)methyl]cyclohexane and 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI) (CA INDEX NAME)

OTHER NAMES:

CN **Bisphenol A diglycidyl ether dimethacrylate-1,4-cyclohexanedimethyl divinyl ether-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer**

MF (C29 H36 O8 . C20 H30 O4 . C12 H20 O2)x

CI PMS

PCT Polyacrylic, Polyether, Polyether formed, Polyvinyl

SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

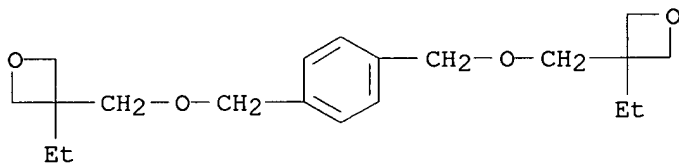
Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	1 in CM 1 2 in CM 3
C6	C6	6	C6	46.150.1	1 in CM 2
C3O	OC3	4	C3O	4.214.1	2 in CM 1

CM 1

CRN 142627-97-2

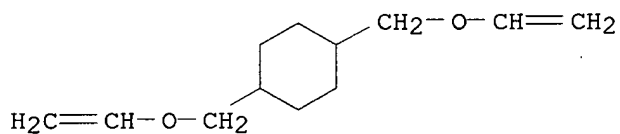
CMF C20 H30 O4



CM 2

CRN 17351-75-6

CMF C12 H20 O2



CM 3

CRN 1565-94-2

CMF C29 H36 O8

REFERENCE 1

ACCESSION NUMBER:	141:54808 CA
TITLE:	Photopolymerization initiator and visible light photopolymerizable composition
INVENTOR(S):	Suzuki, Takeshi; Kazama, Hideki
PATENT ASSIGNEE(S):	Tokuyama Corporation, Japan; Tokuyama Dental Corporation
SOURCE:	Eur. Pat. Appl., 33 pp. CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	English
INT. PATENT CLASSIF.:	
MAIN:	C08F002-50
SECONDARY:	C08G059-00; A61K006-00
CLASSIFICATION:	35-3 (Chemistry of Synthetic High Polymers) Section cross-reference(s): 63
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1431315	A2	20040623	EP 2003-258015	20031218
EP 1431315	A3	20041013		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004196949	A2	20040715	JP 2002-367080	20021218
US 2004186195	A1	20040923	US 2003-737827	20031218
PRIORITY APPLN. INFO.:			JP 2002-367080	20021218

The photopolymn. initiator comprises: (A) a photo acid-generating compound such as diaryliodonium salt (e.g., di-Ph iodonium, bis(p-chlorophenyl)iodonium, etc.), (B) a photo oxidation radical-generating compound such as diarylketone compound,  $\alpha$ -diketone compound or ketocoumarin compound, and (C) a fused polycyclic aromatic compound such as 1,4-dimethylnaphthalene, 1-methylantracene, 9-methylantracene, 9,10-dimethylantracene or 9,10-diethylantracene. The photopolymn. initiator makes it possible to efficiently polymerize the cationically polymerizable monomer by the irradiation with visible light and useful for dental cement.

SUPPL. TERM: visible light photopolymerizable compn acid generating photoinitiator; dental cement photopolymerizable oxidn radical generating photoinitiator

INDEX TERM: Dental materials and appliances  
(cements; manufacture of photopolymn. initiator for visible light photopolymerizable composition)

INDEX TERM: Epoxy resins, preparation  
ROLE: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(manufacture of photopolymn. initiator for visible light photopolymerizable composition)

INDEX TERM: Polymerization catalysts  
(photopolymn.; manufacture of photopolymn. initiator for visible light photopolymerizable composition)

INDEX TERM: 57-97-6, 7,12-Dimethylbenz[a]anthracene 571-58-4, 1,4-Dimethylnaphthalene 779-02-2, 9-Methylantracene 781-43-1, 9,10-Dimethylantracene 1468-95-7, 9-Hydroxymethylantracene 1498-71-1, 9-Benzylantracene 1624-32-4, 9,10-Diethylantracene 2584-79-4, 9-Methoxymethylantracene 4766-40-9, 4,5-Dihydrobenz[j]acephenanthrylene 10273-85-5, 9,10-Anthracenedimethanol 23707-65-5, 9-Allylantracene 24463-19-2, 9-Chloromethylantracene 63041-77-0, 7-Methylbenzo[a]pyrene 63226-13-1, 3,3'-Bis(7-diethylaminocoumarinyl) ketone 98178-26-8, 9-(Dimethoxy)methylantracene  
ROLE: CAT (Catalyst use); USES (Uses)  
(manufacture of photopolymn. initiator for visible light photopolymerizable composition)

INDEX TERM: 25085-98-7P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate polymer 25085-99-8P, Bisphenol A diglycidyl ether polymer 26426-05-1P, Bisphenol A diglycidyl ether dimethacrylate; triethylene glycol dimethacrylate copolymer 142627-97-2P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate-4-ethyl-2,6,7-trioxabicyclo[2.2.2]octane copolymer 142675-43-2P, Bis(3-ethyl-3-oxetanylmethyl) ether polymer 151543-64-5P, 1,4-Cyclohexanedimethyl divinyl ether polymer 167488-42-8P, Bisphenol A diglycidyl ether-1,4-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 167488-43-9P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 191611-67-3P, Bis(3-ethyl-3-oxetanylmethyl) ether-3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate copolymer 691883-53-1P, Bis(3-ethyl-3-oxetanylmethyl) ether-bisphenol A diglycidyl ether copolymer 691894-74-3P, Bis(3-ethyl-3-oxetanylmethyl) ether-1,4-cyclohexanedimethyl divinyl ether copolymer 705284-17-9P, Bis(3-ethyl-3-oxetanylmethyl) ether-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 705284-19-1P, Bis(3-ethyl-3-oxetanylmethyl) ether-bisphenol A diglycidyl ether dimethacrylate-3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate copolymer 705284-21-5P, Bisphenol A diglycidyl ether dimethacrylate-3,4-epoxycyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 705284-23-7P, Bis(3-ethyl-3-oxetanylmethyl ether)-bisphenol A diglycidyl ether dimethacrylate-1,4-cyclohexanedimethyl divinyl ether copolymer 705284-25-9P, Bisphenol A diglycidyl ether dimethacrylate-1,4-cyclohexanedimethyl divinyl ether-xylylene glycol di(3-ethyl-3-oxetanylmethyl

ether) copolymer  
 ROLE: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (manufacture of photopolymn. initiator for visible light photopolymerizable composition)  
 INDEX TERM: 52754-92-4, Diphenyliodonium hexafluoroantimonate  
 61358-23-4, Di(4-tert-butylphenyl)iodonium hexafluoroantimonate 87709-41-9  
 ROLE: CAT (Catalyst use); USES (Uses)  
 (photo-acid generator; manufacture of photopolymn. initiator for visible light photopolymerizable composition)  
 INDEX TERM: 84-65-1, Anthraquinone 90-47-1, Xanthone 134-81-6, Dibenzoyl 486-25-9, Fluorenone 492-22-8, Thioxanthone 2498-66-0, 1,2-Benzoanthraquinone 10373-78-1, Camphorquinone  
 ROLE: CAT (Catalyst use); USES (Uses)  
 (radical generator; manufacture of photopolymn. initiator for visible light photopolymerizable composition)

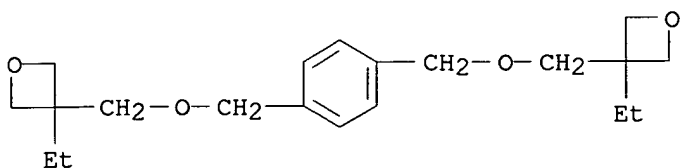
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 RN 705284-21-5 REGISTRY  
 ED Entered STN: 07 Jul 2004  
 CN 7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid, 7-oxabicyclo[4.1.0]hept-3-ylmethyl ester, polymer with (1-methylethylidene)bis[4,1-phenyleneoxy(2-hydroxy-3,1-propanediyl)] bis(2-methyl-2-propenoate) and 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN **Bisphenol A diglycidyl ether dimethacrylate-3,4-epoxycyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer**  
 MF (C29 H36 O8 . C20 H30 O4 . C14 H20 O4)x  
 CI PMS  
 PCT Epoxy resin, Polyacrylic, Polyester, Polyether, Polyether formed  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
=====	=====	=====	=====	=====	=====
C6	C6	6	C6	46.150.18	1 in CM
					1 2 in CM
					3
C20-C6	OC2-C6	3-6	C6O	106.32.1	2 in CM
					2
C30	OC3	4	C3O	4.214.1	2 in CM
					1

CM 1

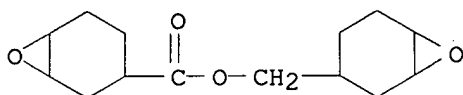
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 CMF C20 H30 O4



CM 2

CRN 2386-87-0

CMF C14 H20 O4

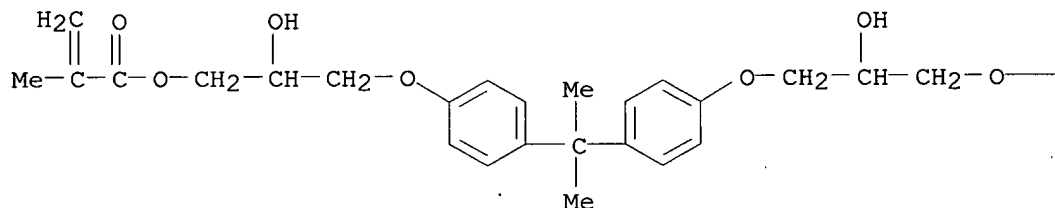


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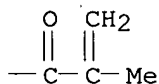
CRN 1565-94-2

CMF C29 H36 O8

PAGE 1-A



PAGE 1-B



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

ACCESSION NUMBER: 141:54808 CA  
TITLE: Photopolymerization initiator and visible light photopolymerizable composition  
INVENTOR(S): Suzuki, Takeshi; Kazama, Hideki  
PATENT ASSIGNEE(S): Tokuyama Corporation, Japan; Tokuyama Dental Corporation  
SOURCE: Eur. Pat. Appl., 33 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English



## INT. PATENT CLASSIF.:

MAIN: C08F002-50  
 SECONDARY: C08G059-00; A61K006-00  
 CLASSIFICATION: 35-3 (Chemistry of Synthetic High Polymers)  
 Section cross-reference(s): 63  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1431315	A2	20040623	EP 2003-258015	20031218
EP 1431315	A3	20041013		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004196949	A2	20040715	JP 2002-367080	20021218
US 2004186195	A1	20040923	US 2003-737827	20031218
PRIORITY APPLN. INFO.:			JP 2002-367080	20021218

## ABSTRACT:

The photopolymn. initiator comprises: (A) a photo acid-generating compound such as diaryliodonium salt (e.g., di-Ph iodonium, bis(p-chlorophenyl)iodonium, etc.), (B) a photo oxidation radical-generating compound such as diarylketone compound,  $\alpha$ -diketone compound or ketocoumarin compound, and (C) a fused polycyclic aromatic compound such as 1,4-dimethylnaphthalene, 1-methylantracene, 9-methylantracene, 9,10-dimethylantracene or 9,10-diethylantracene. The photopolymn. initiator makes it possible to efficiently polymerize the cationically polymerizable monomer by the irradiation with visible light and useful for dental cement.

SUPPL. TERM: visible light photopolymerizable compn acid generating photoinitiator; dental cement photopolymerizable oxidn radical generating photoinitiator  
 INDEX TERM: Dental materials and appliances  
 (cements; manufacture of photopolymn. initiator for visible light photopolymerizable composition)  
 INDEX TERM: Epoxy resins, preparation  
 ROLE: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (manufacture of photopolymn. initiator for visible light photopolymerizable composition)  
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 (photopolymn.; manufacture of photopolymn. initiator for visible light photopolymerizable composition)  
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 ROLE: CAT (Catalyst use); USES (Uses)  
 (manufacture of photopolymn. initiator for visible light photopolymerizable composition)  
 INDEX TERM: 25085-98-7P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate polymer 25085-99-8P, Bisphenol A diglycidyl ether polymer 26426-05-1P, Bisphenol A diglycidyl ether dimethacrylate; triethylene glycol dimethacrylate copolymer 142627-97-2P,

3,4-Epoxy cyclohexylmethyl 3',4'-epoxy cyclohexanecarboxylate-4-ethyl-2,6,7-trioxabicyclo[2.2.2]octane copolymer 142675-43-2P, Bis(3-ethyl-3-oxetanylmethyl) ether polymer 151543-64-5P, 1,4-Cyclohexanedimethyl divinyl ether polymer 167488-42-8P, Bisphenol A diglycidyl ether-1,4-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 167488-43-9P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxy cyclohexanecarboxylate-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 191611-67-3P, Bis(3-ethyl-3-oxetanylmethyl) ether-3,4-Epoxy cyclohexylmethyl 3',4'-epoxy cyclohexanecarboxylate copolymer 691883-53-1P, Bis(3-ethyl-3-oxetanylmethyl) ether-bisphenol A diglycidyl ether copolymer 691894-74-3P, Bis(3-ethyl-3-oxetanylmethyl) ether-1,4-cyclohexanedimethyl divinyl ether copolymer 705284-17-9P, Bis(3-ethyl-3-oxetanylmethyl) ether-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 705284-19-1P, Bis(3-ethyl-3-oxetanylmethyl) ether-bisphenol A diglycidyl ether dimethacrylate-3,4-Epoxy cyclohexylmethyl 3',4'-epoxy cyclohexanecarboxylate copolymer 705284-21-5P, Bisphenol A diglycidyl ether dimethacrylate-3,4-epoxy cyclohexylmethyl 3',4'-epoxy cyclohexanecarboxylate-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 705284-23-7P, Bis(3-ethyl-3-oxetanylmethyl ether)-bisphenol A diglycidyl ether dimethacrylate-1,4-cyclohexanedimethyl divinyl ether copolymer 705284-25-9P, Bisphenol A diglycidyl ether dimethacrylate-1,4-cyclohexanedimethyl divinyl ether-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer

ROLE: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (manufacture of photopolymn. initiator for visible light photopolymerizable composition)

INDEX TERM: 52754-92-4, Diphenyliodonium hexafluoroantimonate 61358-23-4, Di(4-tert-butylphenyl)iodonium hexafluoroantimonate 87709-41-9

ROLE: CAT (Catalyst use); USES (Uses) (photo-acid generator; manufacture of photopolymn. initiator for visible light photopolymerizable composition)

INDEX TERM: 84-65-1, Anthraquinone 90-47-1, Xanthone 134-81-6, Dibenzoyl 486-25-9, Fluorenone 492-22-8, Thioxanthone 2498-66-0, 1,2-Benzoanthraquinone 10373-78-1, Camphorquinone

ROLE: CAT (Catalyst use); USES (Uses) (radical generator; manufacture of photopolymn. initiator for visible light photopolymerizable composition)

L5 ANSWER 4 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 705284-17-9 REGISTRY

ED Entered STN: 07 Jul 2004

CN Oxetane, 3,3'-[oxybis(methylene)]bis[3-ethyl-, polymer with 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI) (CA INDEX NAME)

OTHER NAMES:

CN **Bis(3-ethyl-3-oxetanylmethyl) ether-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer**

MF (C20 H30 O4 . C12 H22 O3)x

CI PMS

PCT. Polyether, Polyether formed

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

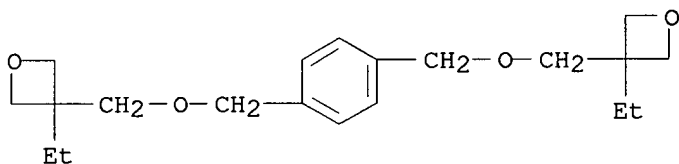
Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3O	OC3	4	C3O	4.214.1	2 in CM
					1 2 in CM
					2
C6	C6	6	C6	46.150.18	1 in CM
					1

CM 1

CRN 142627-97-2

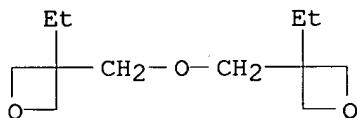
CMF C20 H30 O4



CM 2

CRN 18934-00-4

CMF C12 H22 O3



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 141:54808 CA  
 TITLE: Photopolymerization initiator and visible light photopolymerizable composition  
 INVENTOR(S): Suzuki, Takeshi; Kazama, Hideki  
 PATENT ASSIGNEE(S): Tokuyama Corporation, Japan; Tokuyama Dental Corporation  
 SOURCE: Eur. Pat. Appl., 33 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INT. PATENT CLASSIF.:  
     MAIN: C08F002-50  
     SECONDARY: C08G059-00; A61K006-00  
 CLASSIFICATION: 35-3 (Chemistry of Synthetic High Polymers)

## Section cross-reference(s): 63

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1431315	A2	20040623	EP 2003-258015	20031218
EP 1431315	A3	20041013		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004196949	A2	20040715	JP 2002-367080	20021218
US 2004186195	A1	20040923	US 2003-737827	20031218
			JP 2002-367080	20021218

PRIORITY APPLN. INFO.:

## ABSTRACT:

The photopolymer initiator comprises: (A) a photo acid-generating compound such as diaryliodonium salt (e.g., di-Ph iodonium, bis(p-chlorophenyl)iodonium, etc.), (B) a photo oxidation radical-generating compound such as diarylketone compound,  $\alpha$ -diketone compound or ketocoumarin compound, and (C) a fused polycyclic aromatic compound such as 1,4-dimethylnaphthalene, 1-methylantracene, 9-methylantracene, 9,10-dimethylantracene or 9,10-diethylantracene. The photopolymer initiator makes it possible to efficiently polymerize the cationically polymerizable monomer by the irradiation with visible light and useful for dental cement.

SUPPL. TERM: visible light photopolymerizable compn acid generating photoinitiator; dental cement photopolymerizable oxidn radical generating photoinitiator

INDEX TERM: Dental materials and appliances  
(cements; manufacture of photopolymer initiator for visible light photopolymerizable composition)

INDEX TERM: Epoxy resins, preparation

ROLE: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(manufacture of photopolymer initiator for visible light photopolymerizable composition)

INDEX TERM: Polymerization catalysts  
(photopolymer.; manufacture of photopolymer initiator for visible light photopolymerizable composition)

INDEX TERM: 57-97-6, 7,12-Dimethylbenz[a]anthracene 571-58-4, 1,4-Dimethylnaphthalene 779-02-2, 9-Methylantracene 781-43-1, 9,10-Dimethylantracene 1468-95-7, 9-Hydroxymethylantracene 1498-71-1, 9-Benzylantracene 1624-32-4, 9,10-Diethylantracene 2584-79-4, 9-Methoxymethylantracene 4766-40-9, 4,5-Dihydrobenz[j]acephenanthrylene 10273-85-5, 9,10-Anthracenedimethanol 23707-65-5, 9-Allylantracene 24463-19-2, 9-Chloromethylantracene 63041-77-0, 7-Methylbenzo[a]pyrene 63226-13-1, 3,3'-Bis(7-diethylaminocoumarinyl) ketone 98178-26-8, 9-(Dimethoxy)methylantracene

ROLE: CAT (Catalyst use); USES (Uses)  
(manufacture of photopolymer initiator for visible light photopolymerizable composition)

INDEX TERM: 25085-98-7P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate polymer 25085-99-8P, Bisphenol A diglycidyl ether polymer 26426-05-1P, Bisphenol A diglycidyl ether dimethacrylate; triethylene glycol dimethacrylate copolymer 142627-97-2P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate-4-ethyl-2,6,7-trioxabicyclo[2.2.2]octane copolymer 142675-43-2P, Bis(3-ethyl-3-oxetanylmethyl) ether polymer 151543-64-5P, 1,4-Cyclohexanedimethyl divinyl ether polymer

167488-42-8P, Bisphenol A diglycidyl ether-1,4-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer  
 167488-43-9P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 191611-67-3P, Bis(3-ethyl-3-oxetanylmethyl) ether-3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate copolymer 691883-53-1P, Bis(3-ethyl-3-oxetanylmethyl) ether-bisphenol A diglycidyl ether copolymer 691894-74-3P, Bis(3-ethyl-3-oxetanylmethyl) ether-1,4-cyclohexanedimethyl divinyl ether copolymer 705284-17-9P, Bis(3-ethyl-3-oxetanylmethyl) ether-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 705284-19-1P, Bis(3-ethyl-3-oxetanylmethyl) ether-bisphenol A diglycidyl ether dimethacrylate-3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate copolymer 705284-21-5P, Bisphenol A diglycidyl ether dimethacrylate-3,4-epoxycyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer 705284-23-7P, Bis(3-ethyl-3-oxetanylmethyl ether)-bisphenol A diglycidyl ether dimethacrylate-1,4-cyclohexanedimethyl divinyl ether copolymer 705284-25-9P, Bisphenol A diglycidyl ether dimethacrylate-1,4-cyclohexanedimethyl divinyl ether-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer

ROLE: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (manufacture of photopolymn. initiator for visible light photopolymerizable composition)

INDEX TERM: 52754-92-4, Diphenyliodonium hexafluoroantimonate  
 61358-23-4, Di(4-tert-butylphenyl)iodonium hexafluoroantimonate 87709-41-9

ROLE: CAT (Catalyst use); USES (Uses)  
 (photo-acid generator; manufacture of photopolymn. initiator for visible light photopolymerizable composition)

INDEX TERM: 84-65-1, Anthraquinone 90-47-1, Xanthone 134-81-6, Dibenzoyl 486-25-9, Fluorenone 492-22-8, Thioxanthone 2498-66-0, 1,2-Benzoanthraquinone 10373-78-1, Camphorquinone

ROLE: CAT (Catalyst use); USES (Uses)  
 (radical generator; manufacture of photopolymn. initiator for visible light photopolymerizable composition)

L5 ANSWER 5 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 623900-81-2 REGISTRY

ED Entered STN: 05 Dec 2003

CN Silane, trimethoxy[3-(oxiranylmethoxy)propyl]-, polymer with 2,2'-[1,4-butanediylbis(oxymethylene)]bis[oxirane], Epo Tohto YDPN 638, 2,2'-[methylenebis(4,1-phenyleneoxymethylene)]bis[oxirane] and 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI) (CA INDEX NAME)

OTHER NAMES:

CN **Bisphenol F diglycidyl ether-1,4-butanediol diglycidyl ether-3-glycidoxypropyltrimethoxysilane-OXT 121-Epo Tohto YDPN 638 copolymer**

MF (C20 H30 O4 . C19 H20 O4 . C10 H18 O4 . C9 H20 O5 Si . Unspecified)x

CI PMS

PCT Epoxy resin, Manual component, Polyether, Polyether formed, Polyether

SR CA

LC STN Files: CA, CAPLUS

DT.CA CAPLUS document type: Patent

RL.P Roles from patents: PREP (Preparation); USES (Uses)

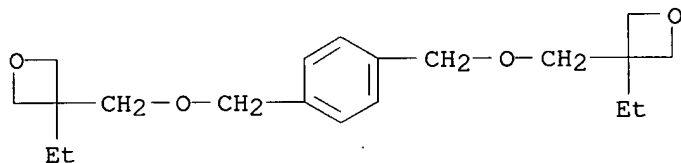
# Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C20	OC2	3	C20	1.30.1	1 in CM 3 2 in CM 4 2 in CM 5
C6	C6	6	C6	46.150.18	1 in CM 1 2 in CM 5
C30	OC3	4	C30	4.214.1	2 in CM 1

CM 1

CRN 142627-97-2

CMF C20 H30 O4



CM 2

CRN 105478-35-1

CMF Unspecified

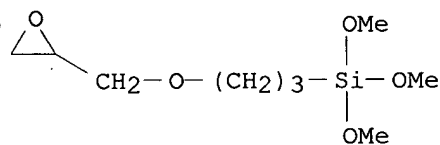
CCI PMS, MAN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

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CRN 2530-83-8

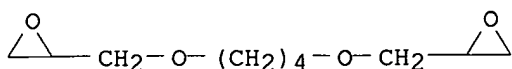
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CM 4

CRN 2425-79-8

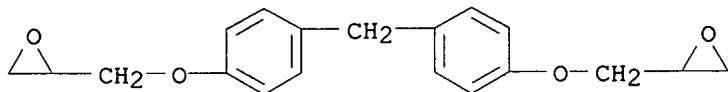
CMF C10 H18 O4



CM 5

CRN 2095-03-6

CMF C19 H20 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

ACCESSION NUMBER: 139:382876 CA  
TITLE: Photocurable resin compositions for moisture-impermeable sealants  
INVENTOR(S): Yamamoto, Yugo; Takamatsu, Yasushi; Sakata, Yoshihiro; Kuwazuka, Toshiaki  
PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
INT. PATENT CLASSIF.:  
MAIN: C09K003-10  
SECONDARY: C08G059-20; C08G065-18; G02F001-1339  
CLASSIFICATION: 42-11 (Coatings, Inks, and Related Products)  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003327951	A2	20031119	JP 2002-135756	20020510
PRIORITY APPLN. INFO.:			JP 2002-135756	20020510

#### ABSTRACT:

Title compns., with 25° viscosity (VS) of 0.01-300 Pa-s, contain oxetane ring-containing compds., epoxy group-containing polycyclic compds., and photo cationic polymerization initiators. A composition comprising OXT 121 49, EP 4088S 15, Rhodorsil 2074 3, SH 6040 3, and talc 30 parts showed VS of 5,000 mPa-s and was photocured to form a film with glass adhesion 35 MPa and moisture permeability 6 g/m<sup>2</sup>-24 h (40°, 90% relative humidity).

SUPPL. TERM: photocurable oxetane polycyclic epoxy compd sealant moisture impermeability; glass adhesion photocurable oxetane polycyclic epoxy compd sealant

INDEX TERM: Phenolic resins, uses  
ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (epoxy, novolak; oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)

INDEX TERM: Sealing compositions  
(oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)

INDEX TERM: Epoxy resins, uses  
ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)

INDEX TERM: Epoxy resins, uses  
ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(phenolic, novolak; oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)

INDEX TERM: 623900-76-5P, Bisphenol F diglycidyl ether-dicyclopentadienediol diglycidyl ether-3-glycidoxypropyltrimethoxysilane-OXT 121 copolymer  
623900-77-6P 623900-78-7P 623900-79-8P, Bisphenol F diglycidyl ether-1,4-butanediol diglycidyl ether-Epo Tohto YDPN 638 copolymer 623900-80-1P 623900-81-2P, Bisphenol F diglycidyl ether-1,4-butanediol diglycidyl ether-3-glycidoxypropyltrimethoxysilane-OXT 121-Epo Tohto YDPN 638 copolymer  
ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(cured; oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)

L5 ANSWER 6 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 623900-76-5 REGISTRY  
ED Entered STN: 05 Dec 2003  
CN Silane, trimethoxy[3-(oxiranylmethoxy)propyl]-, polymer with 2,2'-[methylenebis(4,1-phenyleneoxymethylene)]bis[oxirane], 2,2'-[(octahydro-4,7-methano-1H-indene-5,?-diyl)bis(methyleneoxymethylene)]bis[oxirane] and 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI) (CA INDEX NAME)

OTHER NAMES:  
CN **Bisphenol F diglycidyl ether-dicyclopentadienediol diglycidyl ether-3-glycidoxypropyltrimethoxysilane-OXT 121 copolymer**  
MF (C20 H30 O4 . C19 H20 O4 . C18 H28 O4 . C9 H20 O5 Si)x  
CI PMS  
PCT Epoxy resin, Polyether, Polyether formed, Polyether  
SR CA  
LC STN Files: CA, CAPLUS  
DT.CA CAPLUS document type: Patent  
RL.P Roles from patents: PREP (Preparation); USES (Uses)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C20	OC2	3	C20	1.30.1	2 in CM
					2 1 in CM
					3 2 in CM
					4

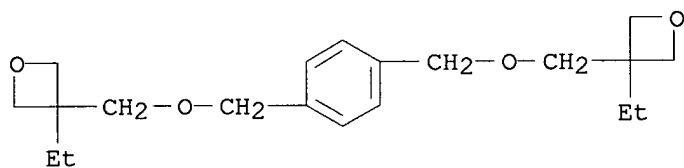


C6	C6	6	C6	46.150.18	1 in CM
					1 2 in CM
					4
C5-C5-C5	C5-C5-C5	5-5-5	C10	553.3.1	1 in CM
					2
C30	OC3	4	C30	4.214.1	2 in CM
					1

CM 1

CRN 142627-97-2

CMF C20 H30 O4

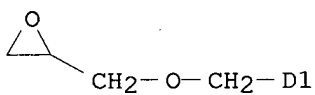
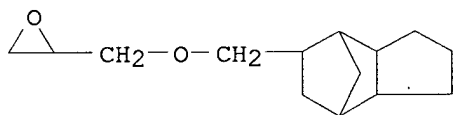


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CRN 50985-55-2

CMF C18 H28 O4

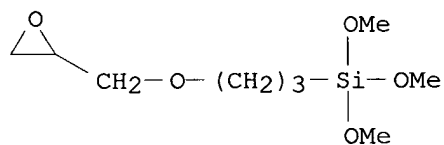
CCI IDS



CM 3

CRN 2530-83-8

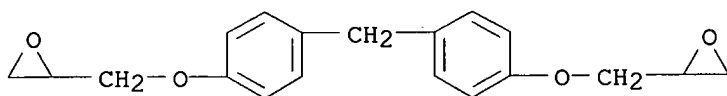
CMF C9 H20 O5 Si



CM 4

CRN 2095-03-6

CMF C19 H20 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

ACCESSION NUMBER: 139:382876 CA  
TITLE: Photocurable resin compositions for moisture-impermeable sealants  
INVENTOR(S): Yamamoto, Yugo; Takamatsu, Yasushi; Sakata, Yoshihiro; Kuwazuka, Toshiaki  
PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
INT. PATENT CLASSIF.:  
MAIN: C09K003-10  
SECONDARY: C08G059-20; C08G065-18; G02F001-1339  
CLASSIFICATION: 42-11 (Coatings, Inks, and Related Products)  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003327951	A2	20031119	JP 2002-135756	20020510
PRIORITY APPLN. INFO.:			JP 2002-135756	20020510

## ABSTRACT:

Title compns., with 25° viscosity (VS) of 0.01-300 Pa-s, contain oxetane ring-containing compds., epoxy group-containing polycyclic compds., and photo cationic polymerization initiators. A composition comprising OXT 121 49, EP 4088S 15, Rhodorsil 2074 3, SH 6040 3, and talc 30 parts showed VS of 5,000 mPa-s and was photocured to form a film with glass adhesion 35 MPa and moisture permeability 6 g/m<sup>2</sup>-24 h (40°, 90% relative humidity).

SUPPL. TERM: photocurable oxetane polycyclic epoxy compd sealant moisture impermeability; glass adhesion photocurable oxetane polycyclic epoxy compd sealant  
INDEX TERM: Phenolic resins, uses  
ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (epoxy, novolak; oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)  
INDEX TERM: Sealing compositions (oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)  
INDEX TERM: Epoxy resins, uses  
ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)

INDEX TERM: Epoxy resins, uses  
 ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (phenolic, novolak; oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)

INDEX TERM: 623900-76-5P, Bisphenol F diglycidyl ether-dicyclopentadienediol diglycidyl ether-3-glycidoxypropyltrimethoxysilane-OXT 121 copolymer 623900-77-6P 623900-78-7P 623900-79-8P, Bisphenol F diglycidyl ether-1,4-butanediol diglycidyl ether-Epo Tohto YDPN 638 copolymer 623900-80-1P 623900-81-2P, Bisphenol F diglycidyl ether-1,4-butanediol diglycidyl ether-3-glycidoxypropyltrimethoxysilane-OXT 121-Epo Tohto YDPN 638 copolymer  
 ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (cured; oxetane-, cationic polymerization initiator-, and polycyclic epoxy compound-containing photocurable sealants with high adhesion and low moisture permeability)

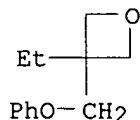
L5 ANSWER 7 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 509107-21-5 REGISTRY  
 ED Entered STN: 02 May 2003  
 CN 7-Oxabicyclo[4.1.0]heptane, polymer with 3-ethyl-3-(phenoxymethyl)oxetane (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN **Cyclohexene oxide-3-ethyl-3-oxetanylmethyl phenyl ether copolymer**  
 MF (C12 H16 O2 . C6 H10 O)x  
 CI PMS  
 PCT Polyether, Polyether formed  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAPLUS document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation)

# Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C20-C6	OC2-C6	3-6	C6O	106.32.1	1 in CM
					2
C3O	OC3	4	C3O	4.214.1	1 in CM
					1
C6	C6	6	C6	46.150.18	1 in CM
					1

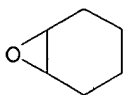
CM 1

CRN 3897-65-2  
 CMF C12 H16 O2



CM 2

CRN 286-20-4  
CMF C6 H10 O



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 138:304641 CA  
TITLE: Monitoring photopolymerization reactions with optical pyrometry  
AUTHOR(S): Falk, Benjamin; Vallinas, Santiago M.; Crivello, James V.  
CORPORATE SOURCE: Department of Chemistry, New York State Center for Polymer Synthesis, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA  
SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (2003), 41(4), 579-596  
CODEN: JPACEC; ISSN: 0887-624X  
PUBLISHER: John Wiley & Sons, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)  
ABSTRACT:

This article describes the development of optical pyrometry (OP) as a new anal. technique for the continuous monitoring of the progress of both free-radical and cationic photopolymns. The method is rapid, reproducible, and very easy to implement. A temperature profile of a photopolymn. can be obtained. Preliminary studies have shown that the temps. of some polymerizing monomers can easily reach temps. in excess of 250 °C. The effects of the mass and reactivity of the monomer, light intensity, structures, and concns. of the photoinitiators and monomers as well as the presence or absence of oxygen on various free-radical and cationic photopolymns. were examined with this method. Coupling of real-time IR spectroscopy with OP provides a convenient method for simultaneously monitoring both the chemical conversion and the temperature of a photopolymn. This combined technique affords new insights into the effects of temperature-induced autoacceleration on the course of photopolymns.

SUPPL. TERM: photopolymn monitoring optical pyrometry  
INDEX TERM: Pyrometry  
(optical; monitoring of photopolymn. by optical pyrometry)  
INDEX TERM: Polymerization  
(photopolymn.; monitoring of photopolymn. by optical pyrometry)  
INDEX TERM: 25085-98-7P, 3,4-Epoxy cyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate homopolymer 25086-25-3P, 4-Vinylcyclohexene dioxide homopolymer 25702-20-9P, Cyclohexene oxide homopolymer 25721-76-0P, Ethylene glycol dimethacrylate homopolymer 28182-75-4P, Diethylene glycol diacrylate homopolymer 31667-45-5P, Triethylene glycol divinyl ether homopolymer 57592-67-3P, 1,6-Hexanediol diacrylate homopolymer 106980-37-4P, Bisphenol A

diacrylate homopolymer 121225-97-6P, PC 1000  
142675-43-2P, Bis(3-Ethyl-3-oxetanylmethyl) ether  
homopolymer 146247-32-7P 153210-03-8P, 1,6-Hexanediol  
divinyl ether homopolymer 167499-43-6P,  
3-Ethyl-3-oxetanylmethyl phenyl ether homopolymer  
509107-21-5P, Cyclohexene oxide-3-Ethyl-3-oxetanylmethyl  
phenyl ether copolymer

ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(monitoring of photopolymn. by optical pyrometry)

REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS  
RECORD.

REFERENCE(S): (1) Akhtar, S; J Org Chem 1990, V55, P4222 CAPLUS  
(2) Anon; Handbook of Chemistry and Physics, 63rd ed 1983,  
PE-385  
(3) Anseth, K; J Polym Sci Part A: Polym Chem 1994, V32,  
P139 CAPLUS  
(4) Anseth, K; Macromolecules 1994, V35, P3243 CAPLUS  
(5) Anseth, K; Polymer 1994, V27, P650 CAPLUS  
(6) Brandrup, J; Polymer Handbook 1965, PE-1  
(7) Brandrup, J; Polymer Handbook 1965, PII-370  
(8) Brandrup, J; Polymer Handbook 1965, PIII  
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L5 ANSWER 8 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 330432-38-7 REGISTRY

ED Entered STN: 06 Apr 2001

CN 7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid, 7-oxabicyclo[4.1.0]hept-3-ylmethyl ester, polymer with 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane], phenylmethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Oxetane, 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyl-, polymer with 7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane-3-carboxylate, phenylmethyl ester (9CI)

OTHER NAMES:

CN **7-Oxabicyclo[4.1.0]hept-3-ylmethyl ester-7-oxabicyclo[4.1.0]heptane-3-carboxylic acid-3,3'-[1,4-phenylene-bis(methyleneoxymethylene)]bis(3-ethyloxetane) copolymer benzyl ether**

MF (C20 H30 O4 . C14 H20 O4)x . x C7 H8 O

PCT Epoxy resin, Polyester, Polyether, Polyether formed  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAPLUS document type: Patent  
 RL.P Roles from patents: PREP (Preparation); USES (Uses)

# Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	1 in CM
					1 1 in CM
					3
C20-C6	OC2-C6	3-6	C6O	106.32.1	2 in CM
					4
C30	OC3	4	C3O	4.214.1	2 in CM
					3

CM 1

CRN 100-51-6

CMF C7 H8 O

HO-CH<sub>2</sub>-Ph

CM 2

CRN 167488-43-9

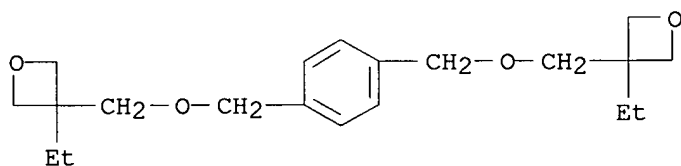
CMF (C20 H30 O4 . C14 H20 O4) x

CCI PMS

CM 3

CRN 142627-97-2

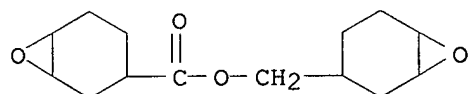
CMF C20 H30 O4



CM 4

CRN 2386-87-0

CMF C14 H20 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 134:238345 CA  
TITLE: UV-curable compositions containing oxetanes and cycloaliphatic epoxy compounds and multifunctional hydroxy compounds and their manufacture  
INVENTOR(S): Hatton, Kevin Brian  
PATENT ASSIGNEE(S): Vantico A.-G., Switz.  
SOURCE: PCT Int. Appl., 26 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
INT. PATENT CLASSIF.:  
MAIN: C08G065-18  
SECONDARY: C08G059-24; C08G059-62  
CLASSIFICATION: 37-6 (Plastics Manufacture and Processing)  
Section cross-reference(s): 38, 42  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019895	A1	20010322	WO 2000-EP8748	20000907
W: AU, CA, JP, KR, US, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 546322	B	20030811	TW 2000-89116197	20000811
CA 2384176	AA	20010322	CA 2000-2384176	20000907
EP 1232198	A1	20020821	EP 2000-960620	20000907
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
JP 2003509553	T2	20030311	JP 2001-523670	20000907
AU 771573	B2	20040325	AU 2000-72850	20000907
ZA 2002002149	A	20030311	ZA 2002-2149	20020315
PRIORITY APPLN. INFO.:			GB 1999-21779	19990916
			WO 2000-EP8748	20000907

ABSTRACT:

The composition, useful for adhesives, coatings, laminating and casting resins, molding compns., putties and sealing compds., comprises (a)  $\geq 1$  oxetane compound; (b)  $\geq 1$  polyfunctional cycloaliph. epoxy compound; (c)  $\geq 1$  multifunctional hydroxy compound; and (d)  $\geq 1$  curing agent. Thus, 88 parts 3,3-[1,4-phenylene-bis(methyleneoxymethylene)]bis(3-ethyloxetane) was mixed with 7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane-3-carboxylate 4, tri(propylene glycol) 4 and Cyacure UVI 6990 1 part to give a clear solution which was test in differential photocalorimeter attached on DSC, showing peak exotherm 16.0 W/g.

SUPPL. TERM: oxetane cycloaliph epoxide multifunctional hydroxy UV curable compn  
INDEX TERM: Adhesives  
Coating materials  
Laminated materials  
Potting compositions  
Putty  
Sealing compositions  
(UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. for)  
INDEX TERM: Molded plastics, uses  
ROLE: TEM (Technical or engineered material use); USES (Uses)



(UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. for)

INDEX TERM: Polyethers, preparation  
Polyoxyalkylenes, preparation

ROLE: IMF (Industrial manufacture); POF (Polymer in formulation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(epoxy-polyester-; UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. and their manufacture)

INDEX TERM: Polyesters, preparation

ROLE: IMF (Industrial manufacture); POF (Polymer in formulation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(epoxy-polyether-; UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. and their manufacture)

INDEX TERM: Polyesters, preparation

ROLE: IMF (Industrial manufacture); POF (Polymer in formulation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(epoxy-polyoxyalkylene-; UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. and their manufacture)

INDEX TERM: Crosslinking catalysts  
(photochem.; UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. and their manufacture)

INDEX TERM: Epoxy resins, preparation

ROLE: IMF (Industrial manufacture); POF (Polymer in formulation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(polyester-polyether-; UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. and their manufacture)

INDEX TERM: Epoxy resins, preparation

ROLE: IMF (Industrial manufacture); POF (Polymer in formulation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(polyester-polyoxyalkylene-; UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. and their manufacture)

INDEX TERM: 104558-94-3, Cyracure UVI 6974 104558-95-4, Cyracure UVI 6990

ROLE: CAT (Catalyst use); USES (Uses)  
(UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. and their manufacture)

INDEX TERM: 330218-90-1P 330218-91-2P 330218-92-3P 330218-93-4P  
330218-94-5P 330218-95-6P 330432-38-7P,  
7-Oxabicyclo[4.1.0]hept-3-ylmethyl ester-7-  
oxabicyclo[4.1.0]heptane-3-carboxylic acid-3,3-[1,4-  
phenylene-bis(methyleneoxymethylene)]bis(3-ethyloxetane)  
copolymer benzyl ether

ROLE: IMF (Industrial manufacture); POF (Polymer in formulation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(UV-curable compns. containing oxetanes and cycloaliph. epoxy compds. and multifunctional hydroxy compds. and their manufacture)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD.

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 (2) Fukudome, K; US 5721020 A 1998 CAPLUS  
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 (4) Japan Synthetic Rubber Co Ltd; EP 0848292 A 1998 CAPLUS  
 (5) Jsr Corp; WO 0063272 A 2000 CAPLUS  
 (6) Kansai Paint Co Ltd; JP 11-152441 A 1999, V1999(11)  
 CAPLUS  
 (7) Nippon Kayaku Co Ltd; JP 11-181391 A 1999, V1999(12)  
 CAPLUS

L5 ANSWER 9 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 325744-20-5 REGISTRY

ED Entered STN: 05 Mar 2001

CN 3-Oxetanemethanol, 3-ethyl-, polymer with 2,2'-[[2-ethyl-2-  
 [(oxiranylmethoxy)methyl]-1,3-propanediyl]bis(oxymethylene)]bis[oxirane]  
 and 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane]  
 (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Oxetane, 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyl-,  
 polymer with 3-ethyl-3-oxetanemethanol and 2,2'-[[2-ethyl-2-  
 [(oxiranylmethoxy)methyl]-1,3-propanediyl]bis(oxymethylene)]bis[oxirane]  
 (9CI)

CN Oxirane, 2,2'-[[2-ethyl-2-[(oxiranylmethoxy)methyl]-1,3-  
 propanediyl]bis(oxymethylene)]bis-, polymer with 3-ethyl-3-oxetanemethanol  
 and 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane]  
 (9CI)

OTHER NAMES:

CN **1,4-Bis[(3-ethyl-3-oxetanylmethoxy)methyl]benzene-3-ethyl-3-  
 hydroxymethyloxetane-trimethylolpropane triglycidyl ether copolymer**

MF (C20 H30 O4 . C15 H26 O6 . C6 H12 O2)x

CI PMS

PCT Epoxy resin, Polyether, Polyether formed

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA CAPLUS document type: Patent

RL.P Roles from patents: PREP (Preparation); PRP (Properties); USES (Uses)

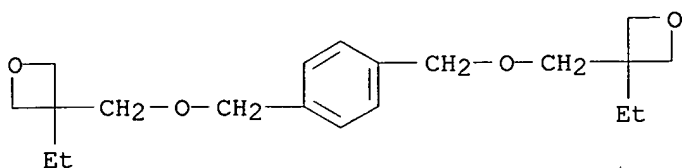
# Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3O	OC3	4	C3O	4.214.1	2 in CM
					1 1 in CM
					3
C2O	OC2	3	C2O	1.30.1	3 in CM
					2
C6	C6	6	C6	46.150.18	1 in CM
					1

CM 1

CRN 142627-97-2

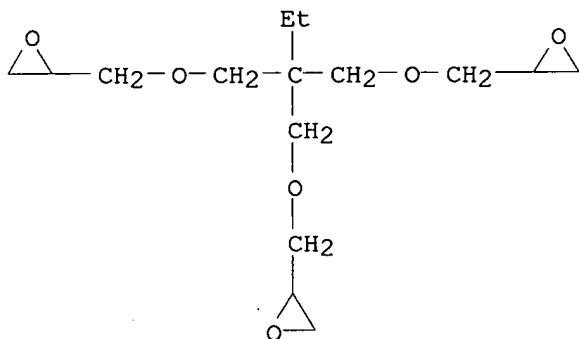
CMF C20 H30 O4



CM 2

CRN 3454-29-3

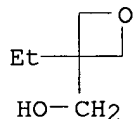
CMF C15 H26 O6



CM 3

CRN 3047-32-3

CMF C6 H12 O2



2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

ACCESSION NUMBER:	134:267848 CA
TITLE:	Oxetanyl compound-containing photocurable encapsulation compositions for electronics and method for their use
INVENTOR(S):	Takamatsu, Yasushi; Nagata, Katsura; Ota, Masahiro; Mizuta, Yasushi; Kikuta, Yoshio
PATENT ASSIGNEE(S):	Mitsui Chemicals Inc., Japan
SOURCE:	Jpn. Kokai Tokkyo Koho, 12 pp. CODEN: JKXXAF
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
INT. PATENT CLASSIF.:	
MAIN:	C09K003-10
SECONDARY:	C09K003-10; G02F001-1339
CLASSIFICATION:	42-11 (Coatings, Inks, and Related Products)

## Section cross-reference(s): 76

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001089743	A2	20010403	JP 1999-270177	19990924
PRIORITY APPLN. INFO.:			JP 1999-270177	19990924

## ABSTRACT:

The compns. providing sealed or encapsulated packages with good heat and moisture resistance, comprise (A) oxetane compds., (B) cationic photoinitiators, (C) silane couplers and (D) inorg. ion exchangers and have viscosity at 25° of 0.01-300 Pa.s. Thus, mixing 1,4-bis[(3-ethyl-3-oxetanylmethoxy)methyl]benzene 70 with 3-ethyl-3-hydroxymethyloxetane 19, 4-PhSC6H4S+Ph2SbF6- 3, 3-glycidoxypropyltrimethoxysilane 3 and IXE 500 (bismuth-type ion exchanger) 5 parts gave a title composition

SUPPL. TERM: cationic photo curable electronic encapsulation compn  
oxetane resin

INDEX TERM: Crosslinking  
(cationic, photochem.; oxetanyl compound-containing photocurable encapsulation compns. for electronics and method for use)

INDEX TERM: Ion exchangers  
(inorg.; oxetanyl compound-containing photocurable encapsulation compns. for electronics and method for use)

INDEX TERM: Coupling agents  
Electronic packaging materials  
(oxetanyl compound-containing photocurable encapsulation compns. for electronics and method for use)

INDEX TERM: Epoxy resins, uses  
ROLE: POF (Polymer in formulation); PRP (Properties); TEM  
(Technical or engineered material use); USES (Uses)  
(oxetanyl compound-containing photocurable encapsulation compns. for electronics and method for use)

INDEX TERM: 71449-78-0, (4-Thiophenoxyphenyl)diphenylsulfonium  
hexafluoroantimonate  
ROLE: CAT (Catalyst use); USES (Uses)  
(cationic photoinitiators; oxetanyl compound-containing photocurable encapsulation compns. for electronics and method for use)

INDEX TERM: 2530-83-8, 3-Glycidoxypropyltrimethoxysilane  
ROLE: MOA (Modifier or additive use); USES (Uses)  
(couplers; oxetanyl compound-containing photocurable encapsulation compns. for electronics and method for use)

INDEX TERM: 137087-38-8, IXE 500 171172-60-4, IXE 550  
ROLE: MOA (Modifier or additive use); USES (Uses)  
(inorg. ion exchanger; oxetanyl compound-containing photocurable encapsulation compns. for electronics and method for use)

INDEX TERM: 210093-34-8, 1,4-Bis[(3-ethyl-3-oxetanylmethoxy)methyl]benzene; 3-ethyl-3-hydroxymethyloxetane copolymer 325744-20-5,  
1,4-Bis[(3-ethyl-3-oxetanylmethoxy)methyl]benzene-3-ethyl-3-hydroxymethyloxetane-trimethylolpropane triglycidyl ether copolymer  
ROLE: POF (Polymer in formulation); PRP (Properties); TEM  
(Technical or engineered material use); USES (Uses)  
(oxetanyl compound-containing photocurable encapsulation compns. for electronics and method for use)

REFERENCE 2

ACCESSION NUMBER: 134:179689 CA  
 TITLE: Photocurable oxetane-containing polymer compositions  
 for packaging flat panels  
 INVENTOR(S): Takamatsu, Yasushi; Nagata, Kei; Ota, Masahiro;  
 Mizuta, Yasushi; Kikuta, Yoshio  
 PATENT ASSIGNEE(S): Mitsui Chemicals, Inc., Japan  
 SOURCE: PCT Int. Appl., 34 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 INT. PATENT CLASSIF.:  
     MAIN: C09K003-10  
     SECONDARY: C08G065-18; C08G059-40; G02F001-1339  
 CLASSIFICATION: 38-3 (Plastics Fabrication and Uses)  
 Section cross-reference(s): 74  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001012745	A1	20010222	WO 2000-JP5329	20000809
W: CN, IN, KR, US, VN				
RW: DE, GB, IT, NL				
EP 1138739	A1	20011004	EP 2000-951911	20000809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2001139933	A2	20010522	JP 2000-249197	20000811
TW 500791	B	20020901	TW 2000-89116320	20000811
US 6586496	B1	20030701	US 2001-787951	20010323
PRIORITY APPLN. INFO.:			JP 1999-228411	19990812
			WO 2000-JP5329	20000809

ABSTRACT:

The composition having viscosity (at 25°) 0.01-300 Pa-s comprises (A) a oxetane ring-containing compound (B) a cationic photopolymer. initiator, (C) a silane coupling agent, and optionally, (D) inorg. filler and (E) epoxy-containing compound  
 The compns. having low-temperature curability, high adhesion strength and good moisture-impermeability are useful for packaging flat panels such as a liquid-crystal display and an electroluminescent display. Thus, 94 parts 1,4-bis[(3-ethyl-3-oxetanylmethoxy)methyl]benzene was mixed with 4-(phenylthio)phenyldiphenylsulfonium hexafluoroantimonate 3 and  $\gamma$ -glycidoxypropyltrimethoxysilane 3 parts, coated between 2 pieces of glass plate and photocured, showing viscosity 134 mPa-s, adhesion strength 8.7 MPa, moisture permeability 20 at 40°, 90% RH and 180 g/m<sup>2</sup>-24 h at 80° 95% RH, resp.

SUPPL. TERM: oxetane polymer packaging liq crystal display; epoxy polyoxyalkylene photocurable electroluminescent display moisture impermeability; cationic polymer catalysts oxetane polymer prepn

INDEX TERM: Polymerization catalysts  
 (cationic, photochem.; photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: Polyoxyalkylenes, uses

ROLE: DEV (Device component use); IMF (Industrial manufacture); POF (Polymer in formulation); PREP (Preparation); USES (Uses)

(epoxy; photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: Coupling agents  
 Electroluminescent devices  
 Electronic packaging materials

Liquid crystal displays  
(photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: Polyoxyalkylenes, uses  
ROLE: DEV (Device component use); IMF (Industrial manufacture); POF (Polymer in formulation); PREP (Preparation); USES (Uses)  
(photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: Epoxy resins, uses  
ROLE: DEV (Device component use); IMF (Industrial manufacture); POF (Polymer in formulation); PREP (Preparation); USES (Uses)  
(polyoxyalkylene-; photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: 71449-78-0  
ROLE: CAT (Catalyst use); USES (Uses)  
(cationic photopolymer. initiator; photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: 178233-72-2  
ROLE: CAT (Catalyst use); USES (Uses)  
(coupling agents; photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: 2530-83-8,  $\gamma$ -Glycidoxypropyltrimethoxysilane  
ROLE: MOA (Modifier or additive use); USES (Uses)  
(coupling agents; photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: 142675-47-6P, 1,4-Bis[(3-ethyl-3-oxetanylmethoxy)methyl]benzene homopolymer 210093-34-8P 325744-19-2P 325744-20-5P 325744-21-6P  
ROLE: DEV (Device component use); IMF (Industrial manufacture); POF (Polymer in formulation); PREP (Preparation); USES (Uses)  
(photocurable oxetane-containing polymer compns. for packaging flat panels)

INDEX TERM: 7631-86-9, Silica, uses  
ROLE: MOA (Modifier or additive use); USES (Uses)  
(photocurable oxetane-containing polymer compns. for packaging flat panels)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Anon; JP 10-168165 A CAPLUS  
(2) Anon; US 5981616 A CAPLUS  
(3) JSR Corporation; EP 848294 A1 1998 CAPLUS  
(4) Nippon Kayaku Co Ltd; JP 10-330717 A 1998 CAPLUS  
(5) Nippon Kayaku Co Ltd; JP 11-209599 A 1999 CAPLUS  
(6) Sony Chemical Corporation; JP 54-3866 A 1993 CAPLUS  
(7) Toagosei Co Ltd; JP 75-3711 A 1995  
(8) Toagosei Co Ltd; JP 11-140279 A 1999 CAPLUS

L5 ANSWER 10 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 324034-07-3 REGISTRY

ED Entered STN: 26 Feb 2001

CN Oxetane, 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyl-, polymer with 3-(methoxymethyl)-3-methyloxetane and [(2-phenoxyethoxy)methyl]oxirane (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Oxetane, 3-(methoxymethyl)-3-methyl-, polymer with [(2-phenoxyethoxy)methyl]oxirane and 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI)

CN Oxirane, [(2-phenoxyethoxy)methyl]-, polymer with 3-(methoxymethyl)-3-methyloxetane and 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-

ethyloxetane] (9CI)  
 OTHER NAMES:  
 CN **Ethylene glycol glycidyl phenyl ether-3-(methoxymethyl)-3-methyloxetane-XDO copolymer**  
 MF (C20 H30 O4 . C11 H14 O3 . C6 H12 O2)x  
 CI PMS  
 PCT Polyether, Polyether formed  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAplus document type: Patent  
 RLD.P Roles for non-specific derivatives from patents: PREP (Preparation);  
 USES (Uses)

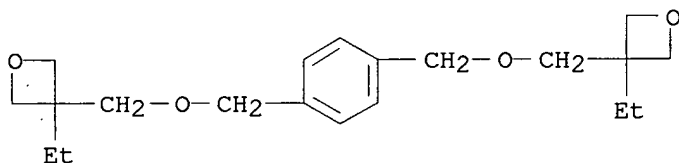
# Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C20	OC2	3	C20	1.30.1	1 in CM 3
C6	C6	6	C6	46.150.18	1 in CM 1 1 in CM 3
C30	OC3	4	C30	4.214.1	2 in CM 1 1 in CM 2

CM 1

CRN 142627-97-2

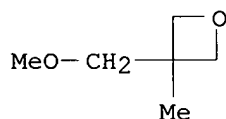
CMF C20 H30 O4



CM 2

CRN 34493-11-3

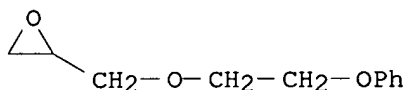
CMF C6 H12 O2



CM 3

CRN 14435-46-2

CMF C11 H14 O3



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 134:156304 CA  
 TITLE: Polymer electrolytes, their manufacture, and electrochemical devices therefrom  
 INVENTOR(S): Sato, Kazuya; Tai, Seiji; Nishiyama, Shino  
 PATENT ASSIGNEE(S): Hitachi Chemical Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 INT. PATENT CLASSIF.:  
     MAIN: H01B001-06  
     SECONDARY: C08G065-18; C08K003-24; C08L071-00; G01N027-406; H01B001-12; H01B013-00; H01M008-02; H01M010-30; H01M010-40  
 CLASSIFICATION: 76-2 (Electric Phenomena)  
                   Section cross-reference(s): 38, 52  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001035250	A2	20010209	JP 1999-205542	19990721
PRIORITY APPLN. INFO.:			JP 1999-205542	19990721

ABSTRACT:

The electrolytes comprise polyethers obtained by reaction of oxetane compds., preferably with epoxy compds. The electrolytes may also contain alkali metal salts. The electrolytes are manufactured by preparation of polyether, by reaction of oxetane compds. in presence of polymerization catalysts, followed by treatment of the polyether with alkali metal salts. Electrochem. devices comprising of thus prepared electrolytes are also claimed.

SUPPL. TERM: polyoxyalkylene lithium complex solid electrolyte; polyether electrolyte manuf electrochem device; battery electrolyte polyoxyalkylene lithium complex; oxetane polymn solid electrolyte manuf  
 INDEX TERM: Electric apparatus  
                   (electrochem., electrolytes; manufacture of polyoxyalkylenes as solid electrolytes for electrochem. devices)  
 INDEX TERM: Battery electrolytes  
                   Polymer electrolytes  
                   (manufacture of polyoxyalkylenes as solid electrolytes for electrochem. devices)  
 INDEX TERM: Polyoxyalkylenes, uses  
                   ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
                   (manufacture of polyoxyalkylenes as solid electrolytes for electrochem. devices)  
 INDEX TERM: 7439-93-2DP, Lithium, polyoxyalkylene complexes, uses



28675-37-8DP, Allyl glycidyl ether-oxetane copolymer,  
lithium complexes, perchlorate-containing 97041-72-0DP,  
lithium complexes, perchlorate-containing 97052-14-7DP,  
lithium complexes, perchlorate-containing 324034-02-8DP,  
Ethylene glycol glycidyl phenyl ether-oxetane copolymer,  
lithium complexes, perchlorate-containing 324034-03-9DP,  
Ethylene glycol glycidyl phenyl ether-3-(methoxymethyl)-3-  
methyloxetane copolymer, lithium complexes,  
perchlorate-containing 324034-04-0DP, lithium complexes,  
perchlorate-containing 324034-05-1DP, 2-(Chloromethyl)oxetane-  
propylene oxide copolymer, lithium complexes,  
perchlorate-containing 324034-06-2DP, 3,3-  
Bis(chloromethyl)oxetane-ethylene oxide copolymer, lithium  
complexes, perchlorate-containing 324034-07-3DP, Ethylene  
glycol glycidyl phenyl ether-3-(methoxymethyl)-3-  
methyloxetane-XDO copolymer, lithium complexes,  
perchlorate-containing 324034-08-4DP, lithium complexes,  
perchlorate-containing

ROLE: IMF (Industrial manufacture); TEM (Technical or  
engineered material use); PREP (Preparation); USES (Uses)  
(manufacture of polyoxyalkylenes as solid electrolytes for  
electrochem. devices)

INDEX TERM: 7791-03-9, Lithium perchlorate 14283-07-9, Lithium  
tetrafluoroborate 21324-40-3, Lithium hexafluorophosphate  
90076-65-6, Lithium bis(trifluoromethanesulfonyl)imide  
ROLE: TEM (Technical or engineered material use); USES (Uses)  
(manufacture of polyoxyalkylenes as solid electrolytes for  
electrochem. devices)

L5 ANSWER 11 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 226091-85-6 REGISTRY

ED Entered STN: 25 Jun 1999

CN 7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid, 7-oxabicyclo[4.1.0]hept-3-  
ylmethyl ester, polymer with 3-ethyl-3-[(hexyloxy)methyl]oxetane,  
3-ethyl-3-oxetanemethanol and 3,3'-[1,4-phenylenebis(methyleneoxymethylene  
)]bis[3-ethyloxetane] (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 3-Oxetanemethanol, 3-ethyl-, polymer with 3-ethyl-3-  
[(hexyloxy)methyl]oxetane, 7-oxabicyclo[4.1.0]hept-3-ylmethyl  
7-oxabicyclo[4.1.0]heptane-3-carboxylate and 3,3'-[1,4-  
phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI)

CN Oxetane, 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyl-,  
polymer with 3-ethyl-3-[(hexyloxy)methyl]oxetane, 3-ethyl-3-  
oxetanemethanol and 7-oxabicyclo[4.1.0]hept-3-ylmethyl  
7-oxabicyclo[4.1.0]heptane-3-carboxylate (9CI)

CN Oxetane, 3-ethyl-3-[(hexyloxy)methyl]-, polymer with 3-ethyl-3-  
oxetanemethanol, 7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-  
oxabicyclo[4.1.0]heptane-3-carboxylate and 3,3'-[1,4-  
phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI)

OTHER NAMES:

CN **3,4-Epoxy cyclohexylmethyl 3,4-epoxycyclohexanecarboxylate-3-ethyl-3-  
hexyloxymethyloxetane-3-ethyl-3-hydroxymethyloxetan-p-xylylene  
bis(ethyloxetanylmethyl) ether copolymer**

MF (C20 H30 O4 . C14 H20 O4 . C12 H24 O2 . C6 H12 O2)x

CI PMS

PCT Epoxy resin, Polyester, Polyether, Polyether formed

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Caplus document type: Patent

RL.P Roles from patents: PREP (Preparation); PRP (Properties); USES (Uses)

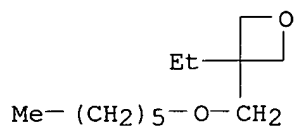
Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C2O-C6	OC2-C6	3-6	C6O	106.32.1	2 in CM 4
C3O	OC3	4	C3O	4.214.1	1 in CM 1 2 in CM 2 1 in CM 3
C6	C6	6	C6	46.150.18	1 in CM 2

CM 1

CRN 226091-84-5

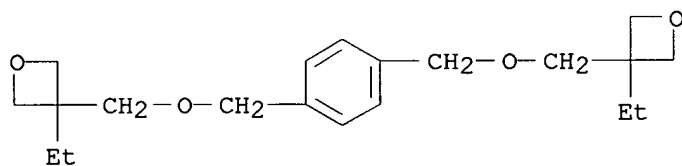
CMF C12 H24 O2



CM 2

CRN 142627-97-2

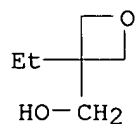
CMF C20 H30 O4



CM 3

CRN 3047-32-3

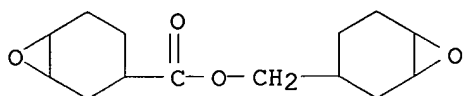
CMF C6 H12 O2



CM 4

CRN 2386-87-0

CMF C14 H20 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 131:20326 CA  
TITLE: Ultraviolet ray-curable coating compositions for cans  
INVENTOR(S): Takami, Seiji  
PATENT ASSIGNEE(S): Kansai Paint Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
INT. PATENT CLASSIF.:  
MAIN: C09D163-00  
SECONDARY: B05D007-14; C09D005-00; C09D007-12; C08G065-08  
CLASSIFICATION: 42-10 (Coatings, Inks, and Related Products)  
Section cross-reference(s): 55  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11152441	A2	19990608	JP 1997-320665	19971121
US 6166101	A	20001226	US 1998-197415	19981123
			JP 1997-320665	19971121

PRIORITY APPLN. INFO.:

ABSTRACT:

Coating materials contain alicyclic epoxy compds. 10-85, oxetane compds. 5-60, compds. having 1 oxetane ring and OH group 5-60, compds. having  $\geq 2$  oxetane rings or an oxetane ring and an epoxy group 5-60, and cationic polymerization catalysts 0.01-20 parts/100 parts above compds. Thus, a coating material for a PET polyester-tin free steel sheet contained 3,4-epoxycyclohexylmethyl 3,4-epoxycyclohexanecarboxylate 40, 3-ethyl-3-hexyloxymethyloxetane 20, 3-ethyl-3-hydroxymethyloxetane 20, and p-xylylene bis(ethyloxetanylmethyl) ether 20, Cyacure UVI 6990 6, decaglycerin laurate wax 0.5, and a silicone wax 0.2 part.

SUPPL. TERM: UV crosslinking coating can; steel can UV curable coating; cationic polymn catalyst coating can; epoxide oxetane coating UV crosslinking

INDEX TERM: Polysiloxanes, uses

ROLE: MOA (Modifier or additive use); USES (Uses)  
(Paintad M, lubricants; UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: Cans

Lubricants

UV radiation

(UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: Epoxides

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: Coating materials

(UV-curable; UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: Polymerization catalysts  
(cationic; UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: Ethers, reactions  
ROLE: RCT (Reactant); RACT. (Reactant or reagent)  
(cyclic; UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: Polymerization catalysts  
(photopolymn.; UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: Polymerization  
(ring-opening; UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: 104558-95-4, Cyracure UVI 6990  
ROLE: CAT (Catalyst use); USES (Uses)  
(Cyracure UVI 6990; UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: 226091-85-6P, 3,4-Epoxy cyclohexylmethyl 3,4-epoxycyclohexanecarboxylate-3-ethyl-3-hexyloxymethyloxetane-3-ethyl-3-hydroxymethyloxetane-p-xylylene bis(ethyloxetanylmethyl) ether copolymer  
ROLE: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: 25167-42-4P, Glycidyl methacrylate-styrene copolymer  
226091-87-8P 226091-89-0P 226091-90-3P 226091-91-4P 226091-92-5P  
ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: 12597-69-2, Steel, uses  
ROLE: TEM (Technical or engineered material use); USES (Uses)  
(UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

INDEX TERM: 125622-15-3, Decaglycerin laurate  
ROLE: MOA (Modifier or additive use); USES (Uses)  
(lubricants; UV ray-curable coating compns. containing epoxides and oxetanes for cans and cationic polymerization catalysts for)

L5 ANSWER 12 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 183292-65-1 REGISTRY

ED Entered STN: 22 Nov 1996

CN Poly(3-oxetanylidene methyleneoxy-1,4-phenylene thio-1,4-phenyleneoxymethylene) (9CI) (CA INDEX NAME)

OTHER NAMES:

CN **3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl thioether copolymer, sru**

CN 3,3-Bis(chloromethyl)oxetane-4,4'-thiodiphenol copolymer sru

CN 3,3-Bis(chloromethyl)oxetane-4,4'-thiodiphenol polymer, sru

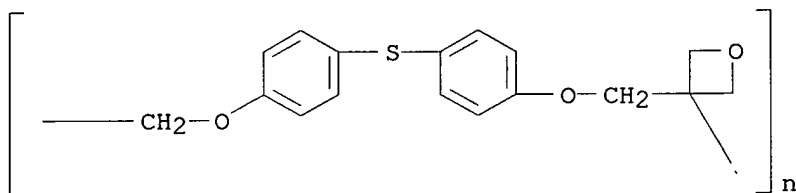
MF (C17 H16 O3 S)n

CI PMS  
 PCT Polyether, Polythioether  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

**\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\***

**Ring System Data**

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
=====	=====	=====	=====	=====	=====
C3O	OC3	4	C3O	4.214.1	1
C6	C6	6	C6	46.150.18	2



4 REFERENCES IN FILE CA (1907 TO DATE)  
 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

**REFERENCE 1**

ACCESSION NUMBER: 136:325944 CA  
 TITLE: Synthesis and modification of oxetane based oligomers with 3-ethoxypropylamine by focused microwave irradiation  
 AUTHOR(S): Baudel, V.; Cazier, F.; Woisel, P.; Surpateanu, G.  
 CORPORATE SOURCE: MREID, Laboratoire de Synthèse Organique et Environnement, Université du Littoral, Dunkerque, 59140, Fr.  
 SOURCE: European Polymer Journal (2002), 38(3), 615-618  
 CODEN: EUPJAG; ISSN: 0014-3057  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)  
 ABSTRACT: Synthesis of oligomers was achieved via condensation of several bisphenol sodium salts in water with 3,3-bis(chloromethyl)oxetane in nitrobenzene under phase transfer catalysis with tetrabutylammonium bromide. All proceedings were developed both by classical and under focused microwave irradiation with complete exptl. parameters control. The rigid oxetane chain was then opened partially with 3-ethoxypropylamine in order to generate some specific properties. Higher substitution was obtained by microwave activation in the presence of the zinc chloride which is well known to react as microwave absorber.  
 SUPPL. TERM: bischloromethyloxetane bisphenol oligomer reaction product ethoxypropylamine; microwave polymn bischloromethyloxetane

bisphenol; oxetane based polyether reaction product  
 ethoxypropylamine  
 INDEX TERM: Polyethers, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (cardo; synthesis and modification of  
 3,3-bis(chloromethyl)oxetane-bisphenol oligomers with  
 3-ethoxypropylamine by focused microwave irradiation)  
 INDEX TERM: Microwave  
 (irradiation; synthesis and modification of  
 3,3-bis(chloromethyl)oxetane-bisphenol oligomers with  
 3-ethoxypropylamine by focused microwave irradiation)  
 INDEX TERM: Polymerization  
 (oligomerization; synthesis and modification of  
 3,3-bis(chloromethyl)oxetane-bisphenol oligomers with  
 3-ethoxypropylamine by focused microwave irradiation)  
 INDEX TERM: Polymerization catalysts  
 (phase-transfer, tetrabutylammonium bromide; synthesis  
 and modification of 3,3-bis(chloromethyl)oxetane-  
 bisphenol oligomers with 3-ethoxypropylamine by focused  
 microwave irradiation)  
 INDEX TERM: Polythioethers  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (polyether-, cardo, oligomeric; synthesis and  
 modification of 3,3-bis(chloromethyl)oxetane-bisphenol  
 oligomers with 3-ethoxypropylamine by focused microwave  
 irradiation)  
 INDEX TERM: Cardo polymers  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (polyether-polythioethers, oligomeric; synthesis and  
 modification of 3,3-bis(chloromethyl)oxetane-bisphenol  
 oligomers with 3-ethoxypropylamine by focused microwave  
 irradiation)  
 INDEX TERM: Cardo polymers  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (polyethers; synthesis and modification of  
 3,3-bis(chloromethyl)oxetane-bisphenol oligomers with  
 3-ethoxypropylamine by focused microwave irradiation)  
 INDEX TERM: Polyethers, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (polythioether-, cardo, oligomeric; synthesis and  
 modification of 3,3-bis(chloromethyl)oxetane-bisphenol  
 oligomers with 3-ethoxypropylamine by focused microwave  
 irradiation)  
 INDEX TERM: 1643-19-2, Tetrabutylammonium bromide  
 ROLE: CAT (Catalyst use); USES (Uses)  
 (catalyst; synthesis and modification of  
 3,3-bis(chloromethyl)oxetane-bisphenol oligomers with  
 3-ethoxypropylamine by focused microwave irradiation)  
 INDEX TERM: 35463-84-4P, 3,3-Bis(chloromethyl)oxetane-bisphenol A  
 copolymer 54180-71-1P 156962-78-6P, 3,3-  
 Bis(chloromethyl)oxetane-4,4'-dihydroxybiphenyl copolymer  
 156962-79-7P 182920-73-6P, 3,3-Bis(chloromethyl)oxetane-  
 4,4'-ethylidenebisphenol copolymer 182920-75-8P  
 182920-82-7P, 3,3-Bis(chloromethyl)oxetane-4,4'-  
 cyclohexylidenebisphenol copolymer 182920-84-9P  
 183292-64-0P, 3,3-Bis(chloromethyl)oxetane-4,4'-thiodiphenol  
 copolymer 183292-65-1P

(Preparation)  
 (polyethers, preparation and structure and properties of)  
 INDEX TERM: Polyethers, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (polyketone-, cardo, preparation and structure and properties of)  
 INDEX TERM: Polyethers, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (polysulfone-, cardo, preparation and structure and properties of)  
 INDEX TERM: Polyethers, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (polythioether-, cardo, preparation and structure and properties of)  
 INDEX TERM: Polyethers, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (thio-, polyether-, cardo, preparation and structure and properties of)  
 INDEX TERM: 35463-84-4P, 3,3-Bis(chloromethyl)oxetane-bisphenol A  
 copolymer 54180-71-1P, 3,3-Bis(chloromethyl)oxetane-  
 bisphenol A copolymer, sru 156962-78-6P,  
 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxybiphenyl  
 copolymer 156962-79-7P 182920-63-4P,  
 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxyazobenzene  
 copolymer 182920-66-7P 182920-73-6P,  
 3,3-Bis(chloromethyl)oxetane-1,1-bis(4-hydroxyphenyl)ethane  
 copolymer 182920-75-8P 182920-77-0P,  
 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenylmethane  
 copolymer 182920-79-2P 182920-82-7P 182920-84-9P  
 182920-86-1P 182920-89-4P 182920-92-9P,  
 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl sulfone  
 copolymer 182920-95-2P, 3,3-Bis(chloromethyl)oxetane-4,4'-  
 dihydroxydiphenyl sulfone copolymer, sru 183292-60-6P,  
 3,3-Bis(chloromethyl)oxetane-1,2-bis(4-hydroxyphenyl)ethane  
 copolymer 183292-61-7P, 3,3-Bis(chloromethyl)oxetane-1,2-  
 bis(4-hydroxyphenyl)ethane copolymer, sru 183292-62-8P,  
 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl ether  
 copolymer 183292-63-9P, 3,3-Bis(chloromethyl)oxetane-4,4'-  
 dihydroxydiphenyl ether copolymer, sru 183292-64-0P,  
 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl  
 thioether copolymer 183292-65-1P, 3,3-  
 Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl thioether  
 copolymer, sru 183292-66-2P, 3,3-Bis(chloromethyl)oxetane-  
 4,4'-dihydroxydiphenyl ketone copolymer 183292-67-3P,  
 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl ketone  
 copolymer, sru 183292-68-4P 183292-69-5P 183292-70-8P  
 183292-71-9P  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (preparation and structure and properties of)

L5 ANSWER 13 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 183292-63-9 REGISTRY

ED Entered STN: 22 Nov 1996

CN Poly(3-oxetanylidene-methyleneoxy-1,4-phenyleneoxy-1,4-  
 phenyleneoxymethylene) (9CI) (CA INDEX NAME)

OTHER NAMES:

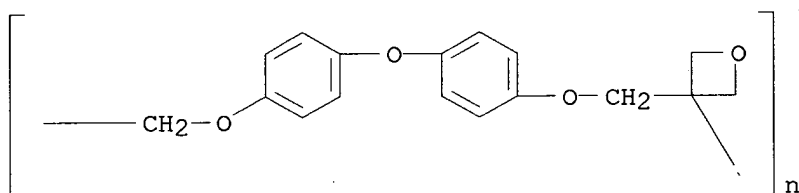
CN 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl ether copolymer,

**sr**  
 MF (C17 H16 O4)n  
 CI PMS  
 PCT Polyether  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP  
 (Properties); RACT (Reactant or reagent)

**\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\***

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3O	OC3	4	C3O	4.214.1	1
C6	C6	6	C6	46.150.18	2



4 REFERENCES IN FILE CA (1907 TO DATE)  
 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 136:310516 CA  
 TITLE: Thermal behavior and primary degradation mechanism of some aromatic polyethers with semi-flexible chain  
 AUTHOR(S): Creanga, A.; Pokol, G.; Hurdac, N.; Novak, Cs.; Alazaroaie, S.; Hurdac, N.  
 CORPORATE SOURCE: Department of Physical and Theoretical Chemistry, A. I. Cuza' University, Iasi, 6600, Rom.  
 SOURCE: Journal of Thermal Analysis and Calorimetry (2001), 66(3), 859-868  
 CODEN: JTACF7; ISSN: 1418-2874  
 PUBLISHER: Kluwer Academic Publishers  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 37-5 (Plastics Manufacture and Processing)  
 ABSTRACT:

The present paper describes a thermogravimetric study combined with mass spectrometry of some aromatic polyethers and copolyethers to obtain information on the degradation mechanism. The studied polymers were synthesized starting from 3,3-bis(chloromethyl) oxetane and various bisphenols: 4,4'-dihydroxyazobenzene, 4,4'-dihydroxydiphenyl, bisphenol A and 4,4'-dihydroxydiphenyl ether. The presence of an oxetane spacer in the structure, permitting the opening of the cycle, induces more complications in the characterization procedure. But, due to the possibilities relative to the modification of polymers or crosslinking



reactions, the presence of the oxetane moiety may offer some advantages. Out of all the studied polymers, those containing azobenzene moieties have the lower thermostability. If the chain flexibility is augmented, the degradation mechanism is based on chain transfer reactions. All polymers present higher thermostability in an argon atmosphere. Based on mass spectra, a degradation mechanism sustained with the assumption that the oxetane unit is the most labile was proposed. The opening of the oxetane cycle begins with the most tensioned bond (-C-CH<sub>2</sub>-) and generates a crosslinking process, which is more evident if the polymer melts below 200°.

SUPPL. TERM: arom polyether primary degradn mechanism thermal behavior  
 INDEX TERM: Polyethers, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (aromatic; thermal behavior and primary degradation mechanism

of

aromatic polyethers)  
 INDEX TERM: Differential thermal analysis  
 (of aromatic polyethers)

INDEX TERM: Polymer degradation  
 Polymer degradation kinetics  
 (thermal; of aromatic polyethers)

INDEX TERM: 1643-19-2, Tetrabutylammonium bromide  
 ROLE: CAT (Catalyst use); USES (Uses)  
 (phase transfer catalyst for preparation of aromatic

polyethers)

INDEX TERM: 35463-84-4P, 3,3-Bis(chloromethyl)oxetane-bisphenol A copolymer 54180-71-1P, 3,3-Bis(chloromethyl)oxetane-bisphenol A copolymer, sru 156962-78-6P, 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl copolymer 156962-79-7P, 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl copolymer, sru 163973-99-7P, 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxyazobenzene copolymer, sru 182920-63-4P, 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxyazobenzene copolymer 183292-62-8P, 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl ether copolymer 183292-63-9P, 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxydiphenyl ether copolymer, sru 202754-48-1P, 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxyazobenzene-4,4'-dihydroxydiphenyl ether copolymer 202754-49-2P, 3,3-Bis(chloromethyl)oxetane-4,4'-dihydroxybiphenyl-4,4'-dihydroxydiphenyl ether copolymer 322471-10-3P, 3,3-Bis(chloromethyl)oxetane-bisphenol A-4,4'-dihydroxydiphenyl ether copolymer  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(thermal behavior and primary degradation mechanism of aromatic polyethers)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD.

- REFERENCE(S):
- (1) Antoun, S; J Polym Sci, Polym Chem Ed 1981, V19, P1901 CAPLUS
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  - (3) Creanga, A; J Therm Anal Cal, in preparation
  - (4) Daoudi, A; J Macromol Sci, Pure Appl Chem 1998, VA35, P151 CAPLUS
  - (5) Hurduc, N; Eur Polym J 1992, V28, P791 CAPLUS
  - (6) Hurduc, N; J Thermal Anal 1996, V47, P735 CAPLUS
  - (7) Hurduc, N; Polym Bull 1992, V28, P639 CAPLUS

(Preparation)

(preparation and structure and properties of)

L5 ANSWER 14 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 182198-91-0 REGISTRY  
ED Entered STN: 22 Oct 1996  
CN Oxetane, 3-ethyl-3-[(phenylmethoxy)methyl]-, homopolymer (9CI) (CA INDEX NAME)

OTHER NAMES:

CN **Poly(3-ethyl-3-hydroxymethyloxetane benzyl ether)**  
MF (C13 H18 O2)x  
CI PMS  
PCT Polyether, Polyether formed  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAPLUS document type: Journal; Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); USES (Uses)  
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

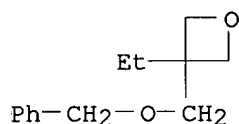
**\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\***

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3O	OC3	4	C3O	4.214.1	1
C6	C6	6	C6	46.150.18	1

CM 1

CRN 18933-99-8  
CMF C13 H18 O2



3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 133:282171 CA  
TITLE: Photochemically induced cationic photopolymerization of vinyl ethers and oxetanes  
AUTHOR(S): Nuyken, O.; Ruile, M.  
CORPORATE SOURCE: Lehrstuhl Makromol. Stoffe, Tech. Univ. Munchen, Garching, D-85747, Germany  
SOURCE: NATO Science Series, Series E: Applied Sciences (1999), 359(Ionic Polymerizations and Related Processes), 117-142  
CODEN: NSSSFC  
PUBLISHER: Kluwer Academic Publishers  
DOCUMENT TYPE: Journal  
LANGUAGE: English

CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)

ABSTRACT:

2,3-Dihydrofuran can be polymerized by means of cationic photoinitiators yielding 100% polymer in less than 120 s at room temperature. The product is colorless, has good film forming properties and does not show any side reaction such as aldehyde formation. Several mono-, bi- and trifunctional oxetanes were synthesized in bulk and in solution cationically. Selected photoinitiators have been applied. It was found that sulfonium salts are very efficient due to good solubility, almost no discoloration of the product and storage stability in the monomer in the absence of light. The conversion was determined by quant. IR-spectroscopy. Conversion between 75% and 85% was found in all cases. The shrinkage during polymerization was much lower than for vinyl monomers. No inhibition by oxygen was observed. Monomer layers thicker than 5.5 mm could be polymerized. The products are transparent and almost colorless. The glass transition temperature of the crosslinked polymers was above 37°C (temperature of the human body).

SUPPL. TERM: photochem cationic polymn vinyl ether oxetane;  
polyoxyalkylene prepn ring opening photopolymn oxetane

INDEX TERM: Polymerization catalysts  
(cationic, photochem.; photochem. induced cationic  
photopolymn. of vinyl ethers and oxetanes)

INDEX TERM: Polymerization catalysts  
Polymerization kinetics  
(cationic, ring-opening; photochem. induced cationic  
photopolymn. of vinyl ethers and oxetanes)

INDEX TERM: Contraction (mechanical)  
Density  
Glass transition temperature  
(photochem. induced cationic photopolymn. of vinyl ethers  
and oxetanes)

INDEX TERM: Polyoxyalkylenes, preparation  
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(photochem. induced cationic photopolymn. of vinyl ethers  
and oxetanes)

INDEX TERM: 74227-35-3, Degacure KI 85B  
ROLE: CAT (Catalyst use); USES (Uses)  
(Degacure KI 85B; photochem. induced cationic  
photopolymn. of vinyl ethers and oxetanes)

INDEX TERM: 142675-47-6P 299162-63-3P  
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(crosslinked; photochem. induced cationic photopolymn. of  
vinyl ethers and oxetanes)

INDEX TERM: 109-63-7 30927-77-6 143084-46-2 143084-48-4  
ROLE: CAT (Catalyst use); USES (Uses)  
(photochem. induced cationic photopolymn. of vinyl ethers  
and oxetanes)

INDEX TERM: 3047-32-3, 3-Ethyl-3-(hydroxymethyl)oxetane 3897-65-2  
18933-99-8, 3-Ethyl-3-hydroxymethyloxetane benzyl ether  
144993-36-2 299162-49-5 299162-53-1 299162-56-4  
299162-60-0  
ROLE: PEP (Physical, engineering or chemical process); PRP  
(Properties); RCT (Reactant); PROC (Process); RACT (Reactant  
or reagent)  
(photochem. induced cationic photopolymn. of vinyl ethers  
and oxetanes)

INDEX TERM: 26221-61-4P, 3-Ethyl-3-hydroxymethyloxetane homopolymer  
30524-28-8P, 3,4-Dihydro-2H-pyran homopolymer 31093-92-2P  
65376-35-4P, 1-Propene, 1-ethoxy-, homopolymer  
75454-45-4P, 2,3-Dihydrofuran homopolymer 167499-43-6P

167499-44-7P 182198-91-0P, Poly(3-ethyl-3-hydroxymethyloxetane benzyl ether) 204767-55-5P  
299162-50-8P 299162-51-9P 299162-52-0P 299162-54-2P  
299162-55-3P 299162-57-5P 299162-59-7P 299162-61-1P  
299162-62-2P

ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(photochem. induced cationic photopolymer. of vinyl ethers  
and oxetanes)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS  
RECORD.

REFERENCE(S): (1) Anon; Organikum 16. Auflage 1986, P269  
(2) Anon; UV-Curing: Science and Technology 1978  
(3) Arnett, E; J Am Chem Soc 1962, V84, P1684 CAPLUS  
(4) Black, P; Can J Chem 1976, V54, P3325 CAPLUS  
(5) Bohner, R; Dissertation, Munchen 1995  
(6) Botteghi, C; Gazz Chim Ital 1975, V105, P233 CAPLUS  
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(8) Crivello, J; Adv Polym Sci 1984, V62, P1 CAPLUS  
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CAPLUS  
(10) Crivello, J; J Macromol Sci, Chem 1993, VA30, P189  
CAPLUS  
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P1473 CAPLUS  
(12) Crivello, J; J Polym Sci: Part A: Polym Chem 1993, V31,  
P1483 CAPLUS  
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P2543 CAPLUS  
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(31) Miyashita, M; J Org Chem 1977, V42, P3772 CAPLUS  
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P751  
(36) Raether, B; Dissertation, TU Munchen 1996  
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(38) Rose, J; J Am Chem Soc 1956, V78, P546  
(39) Sasaki, H; J Macromol Sci, Chem 1992, VA29, P915 CAPLUS  
(40) Shankar, S; US 4400541 1983 CAPLUS  
(41) Stork, G; J Am Chem Soc 1983, V105, P3720 CAPLUS  
(42) Ueno, Y; J Am Chem Soc 1982, V104, P5564 CAPLUS  
(43) Voit, B; Dissertation, Bayreuth 1990  
(44) Yagci, Y; J Polym Sci: Part A: Polym Chem 1992, V30,  
P1987 CAPLUS

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 728790	A1	19960828	EP 1996-101788	19960208
EP 728790	B1	20000503		
R: CH, DE, FR, GB, IT, LI				
DE 19506222	A1	19960829	DE 1995-19506222	19950222
DE 19506222	B4	20041125		
JP 08245783	A2	19960924	JP 1996-33920	19960221
JP 2880446	B2	19990412		
PRIORITY APPLN. INFO.:			DE 1995-19506222 19950222	

## ABSTRACT:

Monomers of specified structure containing oxetane groups are prepared, which give low shrinkage during polymerization and are useful in coatings and as medical and dental materials (no data). Heating equimolar amts. of di-Et carbonate with trimethylolpropane in the presence of KOH at 105-110° for 1 h gave 78% 3-ethyl-3-(hydroxymethyl)oxetane (I). Catalytic photopolymerization of a thin film of I resulted in 7.8% shrinkage; vs. 21.3 for MMA.

SUPPL. TERM: oxetane deriv monomer prepn; shrinkage resistant oxetane monomer; trimethylolpropane reaction ethyl carbonate; ethyloxetanemethanol monomer prepn; coating oxetane deriv monomer; dental material oxetane deriv monomer; surgical material oxetane deriv monomer

INDEX TERM: Monomers

ROLE: IMF (Industrial manufacture); PREP (Preparation)  
(oxetane derivative monomers with low shrinkage in

polymerization)

INDEX TERM: Coating materials

Dental materials and appliances

(oxetane derivative polymers with low shrinkage in

polymerization)

INDEX TERM: Medical goods

(bone cements, oxetane derivative polymers with low shrinkage in polymerization)

INDEX TERM: 18933-99-8P 142627-97-2P

ROLE: IMF (Industrial manufacture); PREP (Preparation)  
(monomers containing oxetane groups)

INDEX TERM: 26221-61-4P 142675-47-6P 182198-91-0P

ROLE: IMF (Industrial manufacture); PREP (Preparation)  
(oxetane derivative polymers with low shrinkage in

polymerization)

INDEX TERM: 3047-32-3P, 3-Ethyl-3-(hydroxymethyl)oxetane

ROLE: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with benzyl halides)

INDEX TERM: 77-99-6, Trimethylolpropane

ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with di-Et carbonate)

INDEX TERM: 100-39-0, Benzyl bromide 623-24-5, 1,4-Bis(bromomethyl)benzene

ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with ethyloxetanemethanol)

INDEX TERM: 105-58-8, Diethyl carbonate

ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with trimethylolpropane)

L5 ANSWER 15 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 167499-43-6 REGISTRY

ED Entered STN: 12 Sep 1995

CN Oxetane, 3-ethyl-3-(phenoxymethyl)-, homopolymer (9CI) (CA INDEX NAME)

## OTHER NAMES:

CN (3-Ethyl-3-oxetanylmethyl) phenyl ether homopolymer

CN 3-Ethyl-3-(phenoxymethyl)oxetane homopolymer

MF (C12 H16 O2)x

CI PMS

PCT Polyether, Polyether formed

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: PREP (Preparation); PRP (Properties); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

## \*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

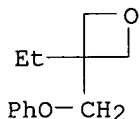
## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3O	OC3	4	C3O	4.214.1	1
C6	C6	6	C6	46.150.18	1

CM 1

CRN 3897-65-2

CMF C12 H16 O2



11 REFERENCES IN FILE CA (1907 TO DATE)

11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

ACCESSION NUMBER: 139:338289 CA

TITLE: Cationic photopolymerization of 2-phenyloxetanes

AUTHOR(S): Kato, Hisao; Sasaki, Hiroshi

CORPORATE SOURCE: Corporate Research Lab, Toagosei Company Ltd., Aichi, 455-0027, Japan

SOURCE: ACS Symposium Series (2003), 847(Photoinitiated Polymerization), 285-295  
CODEN: ACSMC8; ISSN: 0097-6156

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 22

## ABSTRACT:

In cationic polymerization, the polymerizability of oxetanes are known to be high, while the initiation is rather slow, which can be explained by the high-energy barrier for the first ring opening. Due to the stabilizing effect of benzyl groups, the introduction of a Ph group into the 2-position of the oxetane ring might enhance the stability of intermediate in the initiation. Based on this idea, the reactivity of 2-phenyloxetanes (2-phenyl-3,3-dimethyloxetane (HPO) and 2-(4-methoxyphenyl)-3,3-dimethyloxetane (MPO)) was studied using photo-DSC

SOURCE: Tsukuba, 300-33, Japan  
Polymeric Materials Science and Engineering (1995),  
72, 475-6  
CODEN: PMSEDG; ISSN: 0743-0515

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 35-3 (Chemistry of Synthetic High Polymers)

ABSTRACT:  
The cationic photopolymn. of 3-ethyl-3-(phenoxymethyl)oxetane in the presence of diphenyl[4-(phenylthio)phenyl]sulfonium hexafluoroantimonate was investigated. The polymerization mechanism is discussed.

SUPPL. TERM: ethylphenoxymethyloxetane cationic photopolymn; mechanism  
ethylphenoxymethyloxetane cationic photopolymn

INDEX TERM: Polyoxyalkylenes, preparation  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(preparation by photoinitiated cationic polymerization of  
ethyl(phenoxymethyl)oxetane)

INDEX TERM: Polymerization  
(cationic, photochem., mechanism of photoinitiated  
cationic polymerization of ethyl(phenoxymethyl)oxetane)

INDEX TERM: 3897-65-2, 3-Ethyl-3-(phenoxymethyl)oxetane  
ROLE: PEP (Physical, engineering or chemical process); RCT  
(Reactant); PROC (Process); RACT (Reactant or reagent)  
(mechanism of photoinitiated cationic polymerization of)

INDEX TERM: 167499-43-6P, 3-Ethyl-3-(phenoxymethyl)oxetane homopolymer  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(preparation by photoinitiated cationic polymerization)

L5 ANSWER 16 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 167488-43-9 REGISTRY

ED Entered STN: 12 Sep 1995

CN 7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid, 7-oxabicyclo[4.1.0]hept-3-ylmethyl ester, polymer with 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Oxetane, 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyl-, polymer with 7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane-3-carboxylate (9CI)

OTHER NAMES:

CN 1,4-Bis[(3-ethyl-3-oxetanylmethoxy)methyl]benzene-3,4-epoxycyclohexylmethyl 3,4-epoxycyclohexanecarboxylate copolymer

CN **3,4-Epoxycyclohexylmethyl 3',4'-epoxycyclohexanecarboxylate-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer**

MF (C20 H30 O4 . C14 H20 O4)x

CI PMS, COM

PCT Epoxy resin, Polyester, Polyether, Polyether formed

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Caplus document type: Conference; Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation); USES (Uses)

#### Ring System Data

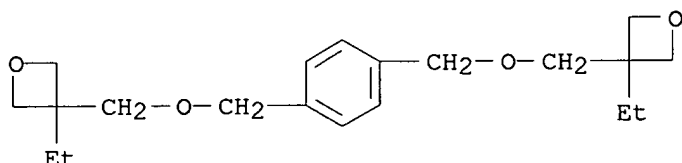
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EA	ES	SZ	RF	RID	Count
C20-C6	OC2-C6	3-6	C6O	106.32.1	2 in CM

C30	OC3	4	C30	4.214.1	2 in CM
C6	C6	6	C6	46.150.18	1 in CM

CM 1

CRN 142627-97-2

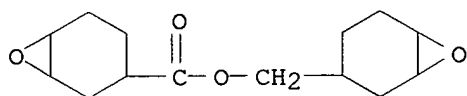
CMF C20 H30 O4



CM 2

CRN 2386-87-0

CMF C14 H20 O4



21 REFERENCES IN FILE CA (1907 TO DATE)

21 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

ACCESSION NUMBER: 141:124053 CA  
 TITLE: Oxetanes: curing properties in photo-cationic polymerization  
 AUTHOR(S): Sasaki, Hiroshi  
 CORPORATE SOURCE: Toagosei Co. Ltd., Japan  
 SOURCE: Experience the World of UV/EB, RadTech 2000: The Premier UV/EB Conference & Exhibition, Technical Conference Proceedings, Baltimore, MD, United States, Apr. 9-12, 2000 (2000), 61-68. RadTech International North America: Chevy Chase, Md.  
 CODEN: 69ETFH  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)  
 ABSTRACT:

Novel oxetane monomers are evaluated in photo-cationic curing system. Monomer with p-methoxyphenyl group on the second position of oxetane ring exhibited high reactivity. In the formulation of oxetanes with cycloaliph. diepoxide monomer, the viscosity of the formulations were reduced, effectively keeping the high surface cure rates of epoxide alone. Difunctional oxetanes exhibited improved solvent resistance.

SUPPL. TERM: photochem cationic polymn oxetane; epoxy resin coating



INDEX TERM: Lenses  
(UV-curable compns. containing oxethanes, epoxy compds., and cationic polymerization initiators for optical material sheets)

INDEX TERM: Epoxy resins, uses  
ROLE: DEV (Device component use); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)  
(alicyclic; UV-curable compns. containing oxethanes, epoxy compds., and cationic polymerization initiators for optical material sheets)

INDEX TERM: Epoxy resins, uses  
ROLE: DEV (Device component use); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)  
(aromatic epoxy resins; UV-curable compns. containing oxethanes, epoxy compds., and cationic polymerization initiators for optical material sheets)

INDEX TERM: Polymerization catalysts  
(cationic; UV-curable compns. containing oxethanes, epoxy compds., and cationic polymerization initiators for optical material sheets)

INDEX TERM: 242488-27-3P  
ROLE: DEV (Device component use); IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process); USES (Uses)  
(UV-curable compns. containing oxethanes, epoxy compds., and cationic polymerization initiators for optical material sheets)

INDEX TERM: 104558-95-4, UVI 6990  
ROLE: CAT (Catalyst use); USES (Uses)  
(initiators; UV-curable compns. containing oxethanes, epoxy compds., and cationic polymerization initiators for optical material sheets)

INDEX TERM: 167488-43-9P 184877-11-0P 225503-83-3P 225503-84-4P 242129-50-6P  
ROLE: DEV (Device component use); IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process); USES (Uses)  
(lens; UV-curable compns. containing oxethanes, epoxy compds., and cationic polymerization initiators for optical material sheets)

L5 ANSWER 17 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 167488-42-8 REGISTRY

ED Entered STN: 12 Sep 1995

CN Oxetane, 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyl-, polymer with 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis[oxirane] (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Oxirane, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-, polymer with 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (9CI)

OTHER NAMES:

CN **Bisphenol A diglycidyl ether-1,4-xylylene glycol di(3-ethyl-3-oxetanylmethyl ether) copolymer**

MF (C21 H24 O4 . C20 H30 O4)x

CI PMS

PCT Epoxy resin, Polyether, Polyether formed

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA CAPLUS document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP

## (Properties); USES (Uses)

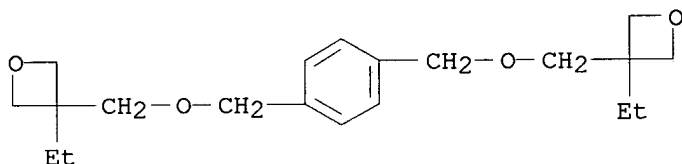
## Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C20	OC2	3	C20	1.30.1	2 in CM 2
C6	C6	6	C6	46.150.18	1 in CM 1 2 in CM 2
C30	OC3	4	C30	4.214.1	2 in CM 1

CM 1

CRN 142627-97-2

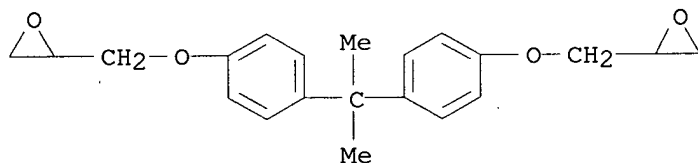
CMF C20 H30 O4



CM 2

CRN 1675-54-3

CMF C21 H24 O4



6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

ACCESSION NUMBER:

142:7357 CA

TITLE:

Active energy curable resin compositions with good curability and low reflectance angle for optical disks

INVENTOR(S):

Makino, Shinji

PATENT ASSIGNEE(S):

Mitsubishi Rayon Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 17 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

INT. PATENT CLASSIF.:

MAIN:

C08G065-04

SECONDARY: G11B007-24  
CLASSIFICATION: 37-6 (Plastics Manufacture and Processing)  
Section cross-reference(s): 38, 42, 74  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004331872	A2	20041125	JP 2003-131585	20030509
PRIORITY APPLN. INFO.:			JP 2003-131585	20030509

ABSTRACT:

Title compns. comprise (A) compds. having  $\geq 2$  oxetane rings, (B) compds. having  $\geq 2$  oxirane rings, (C) cationic photoinitiators, (D) compds. having  $\geq 1$  (meth)acryloyl group, and (E) radical photoinitiators. Thus, a composition comprising OXT 121 25, YD 8125 bisphenol A diglycidyl ether 25, UVI 6990 photoinitiator 3.0, U 2PHA diacrylate 5.0, and Irgacure 184 1.0 parts was applied on a silver-coated Panlite AD 9000TG optical disk and irradiated with a high pressure mercury lamp to give a test piece with reflectance angle  $0.16^\circ$  initially and  $0.06^\circ$  after durability test, transmittance 91% at 400 nm, 93% at 500 nm, and 93% at 700 nm, good surface hardness and reliability.

SUPPL. TERM: active energy curable resin curability reflectance angle  
optical disk; oxetane epoxy copolymer acrylic polymer  
protective coating optical disk

INDEX TERM: Coating materials  
Optical disks

(active energy curable resin compns. with good curability  
and low reflectance angle for optical disks)

INDEX TERM: 167488-42-8P, OXT 121-YD 8125 copolymer

ROLE: IMF (Industrial manufacture); POF (Polymer in  
formulation); PRP (Properties); TEM (Technical or engineered  
material use); PREP (Preparation); USES (Uses)  
(blend with acrylic polymer; active energy curable resin  
compns. with good curability and low reflectance angle  
for optical disks)

INDEX TERM: 115647-57-9P

ROLE: IMF (Industrial manufacture); POF (Polymer in  
formulation); PRP (Properties); TEM (Technical or engineered  
material use); PREP (Preparation); USES (Uses)  
(blend with epoxy resin; active energy curable resin  
compns. with good curability and low reflectance angle  
for optical disks)

INDEX TERM: 24936-68-3, Panlite AD 9000TG, uses

ROLE: TEM (Technical or engineered material use); USES (Uses)  
(substrate; active energy curable resin compns. with good  
curability and low reflectance angle for optical disks)

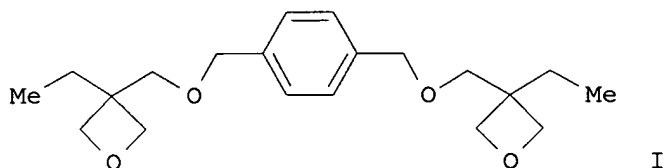
REFERENCE 2

ACCESSION NUMBER: 141:55334 CA  
TITLE: Radiation-curable resin compositions, optical sheets  
from them, and their manufacture  
INVENTOR(S): Makino, Shinji  
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
INT. PATENT CLASSIF.:  
MAIN: C08G065-18  
SECONDARY: C08G059-02; C08J005-18; G02B001-04; G02B005-04;

SECONDARY: C08G059-20; C08G059-40; C08G065-22  
CLASSIFICATION: 37-6 (Plastics Manufacture and Processing)  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07053711	A2	19950228	JP 1993-223820	19930817
PRIORITY APPLN. INFO.:			JP 1993-223820	19930817

GRAPHIC IMAGE:



ABSTRACT:

Title compns. comprise (A) compds. having  $\geq 2$  oxetane rings in a mol., (B) compds. having  $\geq 1$  oxirane ring in a mol., and (C) cationic photopolymn. initiators. Thus, compound I 75, bisphenol A diglycidyl ether 25, and diphenyl-4-thiophenoxyphenylsulfonium hexafluoroantimonate 2.5 parts were mixed to give a composition [viscosity 148 cP (at 25°)], which was coated on a steel plate, cured by UV irradiation, and gave pencil hardness H and good adhesion property and curability.

SUPPL. TERM: oxetane compd curable compn; oxirane compd curable compn  
INDEX TERM: Polymerization catalysts  
(cationic, photochem., active energy ray-curable compns.  
for cured products with good adhesion to base materials)  
INDEX TERM: 71449-78-0  
ROLE: CAT (Catalyst use); USES (Uses)  
(cationic photopolymn. initiator; active energy  
ray-curable compns. for cured products with good adhesion  
to base materials)  
INDEX TERM: 167488-42-8P 167488-43-9P 167488-44-0P 167488-45-1P  
ROLE: IMF (Industrial manufacture); PRP (Properties); TEM  
(Technical or engineered material use); PREP (Preparation);  
USES (Uses)  
(cured product; active energy ray-curable compns. for  
cured products with good adhesion to base materials)

L5 ANSWER 18 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 46129-77-5 REGISTRY

ED Entered STN: 16 Nov 1984

CN Oxetane, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-Oxetanemethyl phenyl ether

FS 3D CONCORD

MF C10 H12 O2

CI COM

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

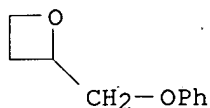
(\*File contains numerically searchable property data)

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C30	OC3	4	C30	4.214.1	1
C6	C6	6	C6	46.150.18	1



#### Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	8.29	pH 1	(1) ACD
Bioconc. Factor (BCF)	8.29	pH 4	(1) ACD
Bioconc. Factor (BCF)	8.29	pH 7	(1) ACD
Bioconc. Factor (BCF)	8.29	pH 8	(1) ACD
Bioconc. Factor (BCF)	8.29	pH 10	(1) ACD
Boiling Point (BP)	254.6+/-13.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	47.21+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	102.1+/-34.9 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	3		(1) ACD
H acceptors (HAC)	2		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	158	pH 1	(1) ACD
Koc (KOC)	158	pH 4	(1) ACD
Koc (KOC)	158	pH 7	(1) ACD
Koc (KOC)	158	pH 8	(1) ACD
Koc (KOC)	158	pH 10	(1) ACD
logD (LOGD)	1.51	pH 1	(1) ACD
logD (LOGD)	1.51	pH 4	(1) ACD
logD (LOGD)	1.51	pH 7	(1) ACD
logD (LOGD)	1.51	pH 8	(1) ACD
logD (LOGD)	1.51	pH 10	(1) ACD
logP (LOGP)	1.511+/-0.248		(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	164.20		(1) ACD
Vapor Pressure (VP)	0.0274064 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

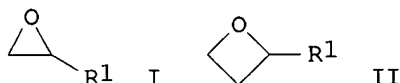
See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 109:92675 CA  
 TITLE: Synthesis of simple oxetanes carrying reactive 2-substituents  
 AUTHOR(S): Fitton, Alan O.; Hill, John; Jane, David E.; Millar, Ross  
 CORPORATE SOURCE: Dep. Chem. Appl. Chem., Univ. Salford, Salford, M5 4WT, UK  
 SOURCE: Synthesis (1987), (12), 1140-2  
 CODEN: SYNTBF; ISSN: 0039-7881  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 27-5 (Heterocyclic Compounds (One Hetero Atom))  
 GRAPHIC IMAGE:



ABSTRACT:

Oxiranes I [ $R_1 = \text{CH}_2\text{OCHMeOEt}$ ,  $\text{CH}_2\text{OCH}_2\text{CH}:\text{CH}_2$ ,  $\text{CH}_2\text{OPh}$ ,  $\text{CH}_2\text{CH}_2\text{CH}:\text{CH}_2$ ,  $\text{CH}(\text{OEt})_2$ ] were treated with  $\text{Me}_2\text{S}^+(\text{O})\text{C}-\text{H}_2$  [from  $\text{Me}_2\text{S}^+(\text{O})\text{Me}$  I- and  $\text{Me}_3\text{COK}$ ] to give the resp. oxetanes II. II ( $R_1 = \text{CH}_2\text{OCHMeOEt}$ ) was hydrolyzed to II ( $R_1 = \text{CH}_2\text{OH}$ ), and the tosylate of the latter and 4- $\text{ClC}_6\text{H}_4\text{SH}$  gave II ( $R_1 = \text{CH}_2\text{SC}_6\text{H}_4\text{Cl}-4$ ).

SUPPL. TERM: oxetanemethanol ether; insertion oxiranemethanol ether  
 oxosulfonium methylide; homologation oxiranemethanol ether  
 oxosulfonium methylide; ring enlargement oxirane  
 INDEX TERM: Insertion reaction  
 (of oxiranemethanol ethers with dimethyloxosulfonium methylide)  
 INDEX TERM: Ring enlargement  
 (of oxiranes, oxetanes by)  
 INDEX TERM: 109-92-2, Ethyl vinyl ether  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (etherification by, of oxiranemethanol)  
 INDEX TERM: 556-52-5, Oxiranemethanol  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (etherification of, by vinyl alkyl ether)  
 INDEX TERM: 106-92-3, Allyl oxiranemethyl ether 122-60-1,  
 Oxiranemethyl phenyl ether 10353-53-4  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (insertion reaction of, with dimethyloxosulfonium methylide)  
 INDEX TERM: 1774-47-6, Trimethyloxosulfonium iodide  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (insertion reaction of, with oxiranemethanol ethers)  
 INDEX TERM: 115785-61-0P  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclocondensation reaction of)  
 INDEX TERM: 4416-85-7P 13269-77-7P, Oxiranecarboxaldehyde diethyl  
 acetal  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and insertion reaction of, with dimethyloxosulfonium methylide)  
 INDEX TERM: 115845-51-7P  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)  
 (preparation and substitution reaction of, with benzenethiol derivative)

INDEX TERM: 46129-77-5P, 2-Oxetanemethyl phenyl ether 61266-70-4P,  
 2-Oxetanemethanol 115845-47-1P 115845-48-2P, Allyl  
 2-oxetanemethyl ether 115845-49-3P 115845-50-6P,  
 2-Oxetancarboxaldehyde diethyl acetal 115845-52-8P  
 115845-53-9P 115845-54-0P 115845-55-1P 115845-56-2P  
 115845-57-3P

ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

INDEX TERM: 106-54-7, 4-Chlorobenzenethiol

ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution reaction of, with oxetanemethyl tosylate)

INDEX TERM: 10487-05-5, 2,3-Dihydroxypropanal diethyl acetal

ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (O-tosylation of)

L5 ANSWER 19 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 30899-38-8 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN Poly(oxy-1,2-ethanediyl),  $\alpha$ -[4-(1,1-dimethylethyl)benzoyl]- $\omega$ -  
 [(3-ethyl-3-oxetanyl)methoxy]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

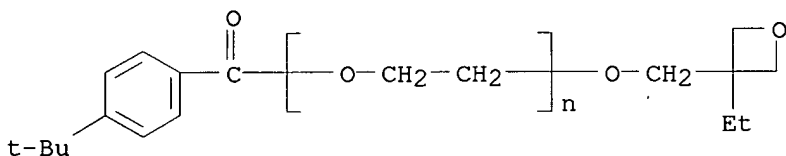
CN **Benzoic acid, p-tert-butyl-, monoester with polyethylene glycol  
 (3-ethyl-3-oxetanyl)methyl ether (8CI)**

CN **Glycols, polyethylene, mono(p-tert-butylbenzoate),  
 (3-ethyl-3-oxetanyl)methyl ether (8CI)**

MF (C2 H4 O)<sub>n</sub> C17 H24 O3  
 CI PMS  
 PCT Polyether  
 LC STN Files: CA, CAPLUS  
 DT.CA CAPLUS document type: Patent  
 RL.P Roles from patents: USES (Uses)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
=====	-----	-----	-----	-----	-----
C3O	OC3	4	C3O	4.214.1	1
C6	C6	6	C6	46.150.18	1



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 73:131924 CA

TITLE: Polyether polyol carboxylates  
 INVENTOR(S): Rudolph, Hans; Langmann, Werner  
 PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.  
 SOURCE: Ger. Offen., 12 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 INT. PATENT CLASSIF.: C08G; B01F  
 CLASSIFICATION: 39 (Textiles)  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1911328	A	19701001	DE 1969-1911328	19690306
PRIORITY APPLN. INFO.:			DE 1969-1911328	19690306

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

ABSTRACT:

The title compds., useful as emulsifiers and dispersing agents (especially for dyes), were prepared by reaction of oxyethylenated [with ethylene oxide (I)] polymers of II, where R = Me or Et (III), with oleic acid (IV), lauric acid, or p-tert-BuC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H. Thus, 140 parts polymerized III, reacted with 6 moles I per OH group, 56.4 parts IV, and 350 parts xylene were refluxed and H<sub>2</sub>O and xylene distilled to give 192 parts ester (V) of 10 acid number. The dye C.I. 12100 (0.5 g) and 1 g V gave a stable aqueous dispersion.

SUPPL. TERM: polyether polyol carboxylates emulsifiers; polyol polyether carboxylates emulsifiers; carboxylates polyether polyol emulsifiers; emulsifiers polyether polyol carboxylates; dyes dispersing agents; dispersing agents dyes; esters polyether polyols

INDEX TERM: Dyes  
 (emulsifying agents for, oxyethylated oxetane derivs. as)

INDEX TERM: Dispersing agents  
 Emulsifying agents  
 (oxyethylated oxetane derivs., for dyes)

INDEX TERM: 30899-37-7 30899-38-8 31116-03-7 31724-01-3

ROLE: USES (Uses)  
 (emulsifying agents, for dyes)

L5 ANSWER 20 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 18933-99-8 REGISTRY

ED Entered STN: 16 Nov 1984

CN Oxetane, 3-ethyl-3-[(phenylmethoxy)methyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Oxetane, 3-[(benzyloxy)methyl]-3-ethyl- (8CI)

OTHER NAMES:

CN 3-(Benzyloxymethyl)-3-ethyloxetane

CN **3-Ethyl-3-hydroxymethyloxetane benzyl ether**

CN [(3-Ethyl-3-oxetanylmethoxy)methyl]benzene

FS 3D CONCORD

MF C13 H18 O2

CI COM

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

DT.CA Caplus document type: Journal; Patent

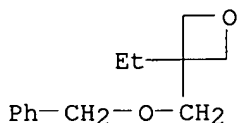
RL.P Roles from patents: PREP (Preparation); PRP (Properties); RACT  
 (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP  
 (Properties); RACT (Reactant or reagent)

Ring System Data



Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3O	OC3	4	C3O	4.214.1	1
C6	IC6	6	IC6	46.150.18	1



#### Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	55.1	pH 1	(1) ACD
Bioconc. Factor (BCF)	55.1	pH 4	(1) ACD
Bioconc. Factor (BCF)	55.1	pH 7	(1) ACD
Bioconc. Factor (BCF)	55.1	pH 8	(1) ACD
Bioconc. Factor (BCF)	55.1	pH 10	(1) ACD
Boiling Point (BP)	280.4+/-13.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (Hvap)	49.83+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	101.8+/-34.9 deg C		(1) ACD
H acceptors (HAC)	2		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	614	pH 1	(1) ACD
Koc (KOC)	614	pH 4	(1) ACD
Koc (KOC)	614	pH 7	(1) ACD
Koc (KOC)	614	pH 8	(1) ACD
Koc (KOC)	614	pH 10	(1) ACD
logD (LOGD)	2.59	pH 1	(1) ACD
logD (LOGD)	2.59	pH 4	(1) ACD
logD (LOGD)	2.59	pH 7	(1) ACD
logD (LOGD)	2.59	pH 8	(1) ACD
logD (LOGD)	2.59	pH 10	(1) ACD
logP (LOGP)	2.594+/-0.293		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	206.28		(1) ACD
Vapor Pressure (VP)	0.00645304 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.67 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.  
18 REFERENCES IN FILE CA (1907 TO DATE)  
18 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD.

- (1) Anon; PATENT ABSTRACTS OF JAPAN 1996, V096(010)
- (2) Ciba Geigy Ag; EP 0732625 A CAPLUS
- (3) Crivello, J; WO 9630182 A CAPLUS
- (4) Ici Plc; EP 0535828 A CAPLUS
- (5) Nuyken, O; MACROMOLECULAR SYMPOSIA 1996, V107, P125 CAPLUS
- (6) Toagosei Co Ltd; JP 08143806 A 1996 CAPLUS

L5 ANSWER 21 OF 21 REGISTRY COPYRIGHT 2005 ACS on STN

RN 3897-65-2 REGISTRY

ED Entered STN: 16 Nov 1984

CN Oxetane, 3-ethyl-3-(phenoxymethyl)- (8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN (3-Ethyl-3-oxetanylmethyl) phenyl ether

CN 3-Ethyl-3-(phenoxymethyl)oxetane

CN Aron Oxetane OXT 211

CN OXT 211

CN POX

CN POX (oxetane)

FS 3D CONCORD

MF C12 H16 O2

CI COM

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, USPATFULL

(\*File contains numerically searchable property data)

DT.CA Caplus document type: Journal; Patent

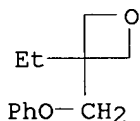
RL.P Roles from patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)

RL.NP Roles from non-patents: PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3O	OC3	4	C3O	4.214.1	1
C6	C6	6	C6	46.150.18	1



#### Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	51.3	pH 1	(1) ACD
Bioconc. Factor (BCF)	51.3	pH 4	(1) ACD
Bioconc. Factor (BCF)	51.3	pH 7	(1) ACD

Bioconc. Factor (BCF)	51.3	pH 8	(1) ACD
Bioconc. Factor (BCF)	51.3	pH 10	(1) ACD
Boiling Point (BP)	274.7+/-13.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	49.25+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	103.8+/-34.9 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	4		(1) ACD
H acceptors (HAC)	2		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	583	pH 1	(1) ACD
Koc (KOC)	583	pH 4	(1) ACD
Koc (KOC)	583	pH 7	(1) ACD
Koc (KOC)	583	pH 8	(1) ACD
Koc (KOC)	583	pH 10	(1) ACD
logD (LOGD)	2.55	pH 1	(1) ACD
logD (LOGD)	2.55	pH 4	(1) ACD
logD (LOGD)	2.55	pH 7	(1) ACD
logD (LOGD)	2.55	pH 8	(1) ACD
logD (LOGD)	2.55	pH 10	(1) ACD
logP (LOGP)	2.553+/-0.263		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	192.25		(1) ACD
Vapor Pressure (VP)	0.00890949 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

51 REFERENCES IN FILE CA (1907 TO DATE)  
17 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
51 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

#### REFERENCE 1

ACCESSION NUMBER: 142:40234 CA  
TITLE: Active ray curable ink-jet ink composition, image forming method using the same, ink-jet recording apparatus, and triarylsulfonium salt compound  
INVENTOR(S): Takabayashi, Toshiyuki; Miura, Norio; Nishizeki, Masato; Okubo, Kimihiko  
PATENT ASSIGNEE(S): Konica Minolta Medical & Graphic, Inc., Japan  
SOURCE: U.S. Pat. Appl. Publ., 55 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
INT. PATENT CLASSIF.:  
MAIN: C07C319-02  
SECONDARY: C07D035-02  
US PATENT CLASSIF.: 106031270  
CLASSIFICATION: 42-12 (Coatings, Inks, and Related Products)  
Section cross-reference(s): 27  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
US 2004244641	A1	20041209	US 2004-826059	20040415

PRIORITY APPLN. INFO.:

JP 2003-116933 20030422  
JP 2003-196367 20030714  
JP 2003-354742 20031015

ABSTRACT:

An active ray curable ink-jet ink composition comprising a photo-induced acid generating agent containing an onium salt which does not generate benzene under active ray radiation, and a photopolymerizable compound containing a compound having an oxetane ring in the mol. Thus, an ink-jet ink composition comprising different color containing PB 822 dispersant, pigment, Celloxide 2021P, Acpress 11M acid amplifier, OP 85R nonionic surfactant, Megafac F 178K surfactant,  $\gamma$ -caprolactone, UVI 6992 photo acid generator, and triarylsulfonium salt was used to print on an oriented polypropylene film, which was irradiated to give a test piece with good print quality and no color mix.

SUPPL. TERM: epoxy resin oxetane deriv photopolymerizable compn inkjet ink; triarylsulfonium salt epoxy resin oxetane deriv photopolymerizable inkjet ink

INDEX TERM: Onium compounds

ROLE: TEM (Technical or engineered material use); USES (Uses)  
(iodonium; photopolymerizable ink-jet ink composition

containing

oxirane or oxetane derivs. and triarylsulfonium salt compound)

INDEX TERM: Inks

(jet-printing; photopolymerizable ink-jet ink composition containing oxirane or oxetane derivs. and triarylsulfonium salt compound)

INDEX TERM: Fatty acids, uses

ROLE: TEM (Technical or engineered material use); USES (Uses)  
(linseed-oil, epoxidized, Me esters; photopolymerizable ink-jet ink composition containing oxirane or oxetane derivs.

and

triarylsulfonium salt compound)

INDEX TERM: Surfactants

(nonionic; active ray curable ink-jet composition, image forming method using the same, ink-jet recording apparatus, and triarylsulfonium salt compound)

INDEX TERM: Epoxy resins, uses

ROLE: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(photopolymerizable ink-jet ink composition containing

oxirane or

oxetane derivs. and triarylsulfonium salt compound)

INDEX TERM: Sulfonium compounds

ROLE: TEM (Technical or engineered material use); USES (Uses)  
(photopolymerizable ink-jet ink composition containing

oxirane or

oxetane derivs. and triarylsulfonium salt compound)

INDEX TERM: Polymerization

(photopolymn.; photopolymerizable ink-jet ink composition containing oxirane or oxetane derivs. and triarylsulfonium salt compound)

INDEX TERM: Fatty acids, uses

ROLE: TEM (Technical or engineered material use); USES (Uses)  
(rape-oil, epoxidized, octyl esters, ADEKACIZER D-55; photopolymerizable ink-jet ink composition containing oxirane

or

oxetane derivs. and triarylsulfonium salt compound)

INDEX TERM: Fatty acids, uses

ROLE: TEM (Technical or engineered material use); USES (Uses)  
(soya, epoxidized, Me esters; photopolymerizable ink-jet

printers)

INDEX TERM: Fatty acids, uses

ROLE: TEM (Technical or engineered material use); USES (Uses)  
 (rape-oil, epoxidized, octyl esters, ADK Cizer D 55, ink  
 containing; actinic ray-curable ink compns. containing

photoacid

generators for jet-printing method and printers)

INDEX TERM: 3897-65-2, OXT 211 18934-00-4, OXT 221 25085-98-7,  
 Celloxide 2021P 29829-07-0, Celloxide 2000 74267-45-1  
 157410-97-4, Sansocizer E-PO 727985-64-0 741292-42-2  
 745041-12-7

ROLE: TEM (Technical or engineered material use); USES (Uses)  
 (ink containing; actinic ray-curable ink compns. containing  
 photoacid generators for jet-printing method and  
 printers)

INDEX TERM: 104558-95-4, UVI 6990 205944-57-6, SP 152 745055-09-8,  
 Chivacure 9842

ROLE: CAT (Catalyst use); USES (Uses)  
 (photoacid generator; actinic ray-curable ink compns.  
 containing photoacid generators for jet-printing method and  
 printers)

INDEX TERM: 745041-08-1 745041-09-2 745041-10-5 745041-11-6

ROLE: CAT (Catalyst use); USES (Uses)  
 (sulfonic acid generator; actinic ray-curable ink compns.  
 containing photoacid generators for jet-printing method and  
 printers)

=>

1/7/2005

ANSWER 1 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 455333-00-3 REGISTRY  
 ED Entered STN: 26 Sep 2002  
 CN 2-Propenoic acid, 2-methyl-, (3-ethyl-3-oxetanyl)methyl ester, polymer  
 with 3-(2,5,8,11,14,17,20,23,26,29-decaoxatriacont-1-yl)-3-ethyloxetane  
 and  $\alpha$ -(1-oxo-2-propenyl)- $\omega$ -methoxypoly(oxy-1,2-ethanediyl)  
 (9CI) (CA INDEX NAME)  
 MF (C25 H50 O11 . C10 H16 O3 . (C2 H4 O)n C4 H6 O2)x  
 CI PMS  
 PCT Polyacrylic, Polyether, Polyether formed  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAPLUS document type: Patent  
 RLD.P Roles for non-specific derivatives from patents: PREP (Preparation);  
 USES (Uses)

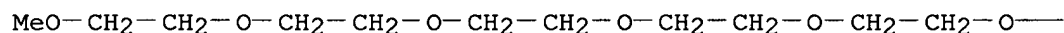
# Ring System Data

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EA	ES	SZ	RF	RID	Count
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					1 1 in CM
					2

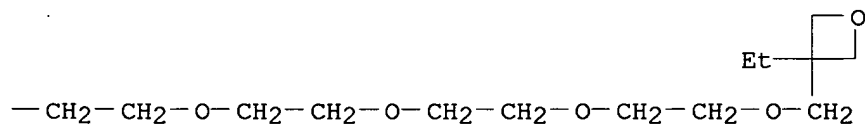
CM 1

CRN 439659-52-6  
 CMF C25 H50 O11

PAGE 1-A

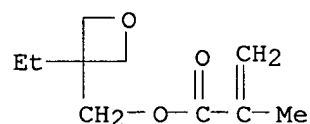


PAGE 1-B



CM 2

CRN 37674-57-0  
 CMF C10 H16 O3

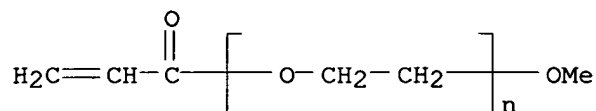


CM 3

CRN 32171-39-4

CMF (C2 H4 O)<sub>n</sub> C4 H6 O2

CCI PMS



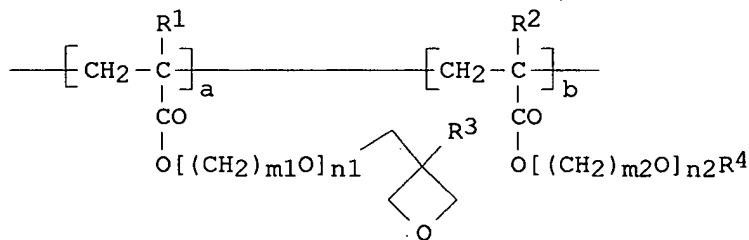
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 137:225156 CA  
TITLE: Oxetane-containing acrylic polymer solid electrolytes and their manufacture  
INVENTOR(S): Miwa, Yoshiyuki  
PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan  
SOURCE: Jpn. Kokai Tokyo Koho, 9 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
INT. PATENT CLASSIF.:  
MAIN: H01B001-06  
SECONDARY: C08F220-28; C08F290-06; C08F299-02; C08G065-22;  
C08K003-00; C08L071-00; H01B001-12; H01B013-00;  
H01G009-035; H01G009-032; H01M006-18; H01M006-22;  
H01M010-40  
CLASSIFICATION: 76-2 (Electric Phenomena)  
Section cross-reference(s): 38  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002260441	A2	20020913	JP 2001-61155	20010306
PRIORITY APPLN. INFO.:			JP 2001-61155	20010306

GRAPHIC IMAGE:



ABSTRACT:

The electrolyte contains electrolyte salt and catalytic ring-opening polymerization product of I (R1-2 = (branched) C1-12 alkyl, H; R3-4 = (branched) C1-12 alkyl;

a, b = 10-600; m1, m2 = 1-6; n1, n2 = 1-20). Markush structures for preferable oxetane comonomers are also given. The electrolytes have excellent film-forming property, flexibility, and high strength. The electrolytes are suitable for use in electrochem. devices.

SUPPL. TERM: oxetane contg acrylic polyoxyalkylene solid electrolyte;  
ring opening polymn oxetane acrylic polyoxyalkylene  
electrolyte; flexible acrylic polyoxyalkylene solid  
electrolyte

INDEX TERM: Polyoxyalkylenes, uses  
ROLE: IMF (Industrial manufacture); TEM (Technical or  
engineered material use); PREP (Preparation); USES (Uses)  
(acrylic; manufacture of flexible acrylic polyoxyalkylene  
solid electrolyte films by ring-opening polymerization of  
oxetane side chains)

INDEX TERM: Polymer electrolytes  
(manufacture of flexible acrylic polyoxyalkylene solid  
electrolyte films by ring-opening polymerization of oxetane  
side  
chains)

INDEX TERM: 3047-32-3P, 3-Ethyl-3-hydroxymethyloxetane 37674-57-0P,  
3-Methacryloxymethyl-3-ethyloxetane  
ROLE: IMF (Industrial manufacture); RCT (Reactant); PREP  
(Preparation); RACT (Reactant or reagent)  
(manufacture of flexible acrylic polyoxyalkylene solid  
electrolyte films by ring-opening polymerization of oxetane  
side  
chains)

INDEX TERM: 7439-93-2DP, Lithium, acrylic polyoxyalkylene complex,  
hexafluorophosphate-containing 455332-98-6DP, lithium complex,  
hexafluorophosphate-containing 455332-99-7DP, lithium complex,  
hexafluorophosphate-containing 455333-00-3DP, lithium complex,  
hexafluorophosphate-containing 455333-01-4DP, lithium complex,  
hexafluorophosphate-containing  
ROLE: IMF (Industrial manufacture); TEM (Technical or  
engineered material use); PREP (Preparation); USES (Uses)  
(manufacture of flexible acrylic polyoxyalkylene solid  
electrolyte films by ring-opening polymerization of oxetane  
side  
chains)

INDEX TERM: 77-99-6, Trimethylolpropane 80-62-6, Methyl methacrylate  
105-58-8, Diethyl carbonate  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(manufacture of flexible acrylic polyoxyalkylene solid  
electrolyte films by ring-opening polymerization of oxetane  
side  
chains)

L2 ANSWER 2 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN

RN 439659-57-1 REGISTRY

ED Entered STN: 21 Jul 2002

CN Oxetane, 3,3'-(2,5,8,11,14-pentaoxapentadecane-1,15-diyl)bis[3-ethyl-,  
polymer with 3-(2,5,8,11,14,17,20,23,26,29-decaoxatriacont-1-yl)-3-  
ethyloxetane (9CI) (CA INDEX NAME)

MF (C25 H50 O11 . C20 H38 O7)x

CI PMS

PCT Polyether, Polyether formed

SR CA

LC STN Files: CA, CAPLUS

DT.CA CAPLUS document type: Journal

RLD.NP Roles for non-specific derivatives from non-patents: PREP  
(Preparation); PRP (Properties)



# Ring System Data

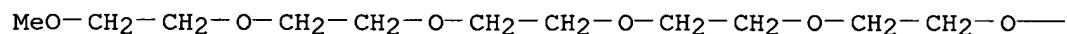
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EA	ES	SZ	RF	RID	Count
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					1 2 in CM
					2

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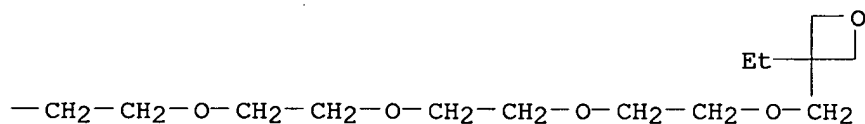
CRN 439659-52-6

CMF C25 H50 O11

PAGE 1-A



PAGE 1-B

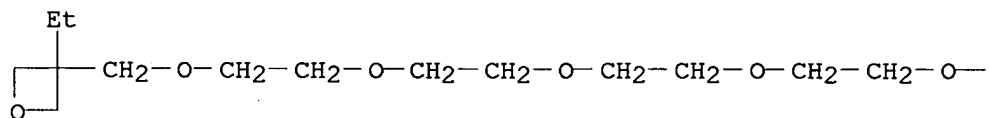


CM 2

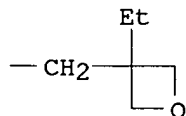
CRN 369404-93-3

CMF C20 H38 O7

PAGE 1-A



PAGE 1-B



- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

ACCESSION NUMBER: 137:63573 CA  
 TITLE: Novel polymer electrolytes based on mono- and bis-oxetane monomers with oligo(ethylene oxide) units  
 AUTHOR(S): Miwa, Yoshiyuki; Tsutsumi, Hiromori; Oishi, Tsutomu  
 CORPORATE SOURCE: Ube Laboratory, Ube Ind. Ltd., Ube, Yamaguchi, 755-8633, Japan  
 SOURCE: Electrochemistry (Tokyo, Japan) (2002), 70(4), 264-269  
 CODEN: EECTFA; ISSN: 1344-3542  
 PUBLISHER: Electrochemical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)  
 Section cross-reference(s): 36, 76

## ABSTRACT:

Polymer electrolytes were prepared by cationic ring-opening polymerization of bis-oxetane (R-O-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>m</sub>-R, R = 3-ethyl-3-methylene oxetane, DDOE (m = 2), TrDOE (m = 3), TeDOE (m = 4)) and mono-oxetane (R-O-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>n</sub>-CH<sub>3</sub>, TrMOE (n = 3), NoMOE (n = 9), DoMOE (n = 12)) with lithium salt catalyst. The polyethers were characterized by differential scanning calorimetry (DSC) and alternating impedance spectroscopy. The poly(oxetane)-based electrolytes have crosslinked networks with oligo(ethylene oxide) and 2-ethyltrimethylene oxide main chains and methoxy-oligo(ethylene oxide) side chains. The polymer electrolytes prepared with LiBF<sub>4</sub> have high ionic conductivity, compared to that of polymers prepared with LiPF<sub>6</sub> or LiN(C<sub>2</sub>F<sub>5</sub>SO<sub>2</sub>)<sub>2</sub>. The conductivity of the poly(oxetane)-LiBF<sub>4</sub> complexes depended on the mono-oxetane content and the length of oligo(ethylene oxide) in the mono- and bis-oxetanes. The oligo(ethylene oxide) side chains in the complexes act as efficient plasticizing agents, particularly NoMOE and DoMOE. Maximum conductivity of the polymer electrolytes with LiBF<sub>4</sub> ([Li]/[O] = 0.045) was 9.1 x 10<sup>-6</sup> (TrMOE/DDOE mole ratio = 3.0) and 1.0 x 10<sup>-4</sup> S-cm<sup>-1</sup> (NoMOE/DDOE = 1.72 and DoMOE/DDOE = 1.29).

SUPPL. TERM: oxetane ring opening polymn polyether prepn lithium salt catalyst; electrolyte polyether oxetane lithium tetrafluoroborate complex cond; ionic cond electrolyte polyether oxetane lithium salt; oligoethylene oxide side chain oxetane polyether glass transition temp

INDEX TERM: Polymerization  
 Polymerization catalysts  
 (cationic, ring-opening; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: Polyoxyalkylenes, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (oxetane-derived; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: Glass transition temperature  
 Ionic conductivity  
 Polymer electrolytes  
 (preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: 383364-44-1P, (3-Ethyl-3-oxetanyl)-2,5,8,11-tetraoxadodecane

439659-52-6P, (3-Ethyl-3-oxetanyl)-  
2,5,8,11,14,17,20,23,26,29-decaoxatriacontane  
439659-53-7P, (3-Ethyl-3-oxetanyl)-  
2,5,8,11,14,17,20,23,26,29,32,35,38-  
tridecaoxanonatriacontane  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(monomer; preparation and ionic conductivity vs. temperature  
of  
oxetane-polyether electrolytes by ring opening polymerization  
with lithium salts as catalysts and counterion source)  
INDEX TERM: 14283-07-9 21324-40-3, Lithium hexafluorophosphate (LiPF<sub>6</sub>)  
132843-44-8, Lithium bis(pentafluoroethylsulfonyl)imide  
ROLE: CAT (Catalyst use); PRP (Properties); USES (Uses)  
(polymerization catalyst and electrolyte; preparation and  
ionic conductivity  
vs. temperature of oxetane-polyether electrolytes by ring  
opening polymerization with lithium salts as catalysts and  
counterion source)  
INDEX TERM: 7439-93-2DP, Lithium, complexes with poly(oxetane-ether)s  
383364-45-2DP, lithium complexes 439659-54-8DP, lithium  
complexes 439659-55-9DP, lithium complexes  
439659-56-0DP, lithium complexes 439659-57-1DP, lithium  
complexes  
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(preparation and ionic conductivity vs. temperature of  
oxetane-polyether  
electrolytes by ring opening polymerization with lithium salts  
as catalysts and counterion source)  
INDEX TERM: 112-35-6, Triethylene glycol monomethyl ether 3047-32-3,  
3-Ethyl-3-hydroxymethyloxetane 5702-16-9, Dodecaethylene  
glycol monomethyl ether 6048-68-6, Nonaethylene glycol  
monomethyl ether  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(preparation and ionic conductivity vs. temperature of  
oxetane-polyether  
electrolytes by ring opening polymerization with lithium salts  
as catalysts and counterion source)  
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
RECORD.  
REFERENCE(S): (1) Abraham, K; Electrochim Acta 1993, V38, P1233 CAPLUS  
(2) Berthier, C; Solid State Ionics 1983, V11, P91 CAPLUS  
(3) Bruce, P; J Chem Soc, Faraday Trans 1993, V89, P3187  
CAPLUS  
(4) Chiang, C; Solid State Ionics 1983, V9 & 10, P1121  
(5) Chovino, C; J Polym Sci, Polym Chem 1997, V35, P2719  
CAPLUS  
(6) Fenton, D; Polymer 1973, V14, P589 CAPLUS  
(7) Harris, S; Macromolecules 1986, V19, P978  
(8) Herogues, V; Macromolecules 1997, V30, P4791  
(9) Killis, A; Macromol Chem Rapid Comm 1980, V1, P595  
CAPLUS  
(10) Miwa, Y; Polym J 2001, V33, P568 CAPLUS  
(11) Miwa, Y; Polym J, in press  
(12) Nishimoto, A; Macromolecules 1999, V32, P1541 CAPLUS  
(13) Papke, B; J Electrochem Soc 1982, V129, P1434 CAPLUS  
(14) Papke, B; J Electrochem Soc 1982, V129, P1694 CAPLUS  
(15) Pattison, D; J Am Chem Soc 1957, V79, P3455 CAPLUS  
(16) Ratner, M; Chem Rev 1988, V88, P109 CAPLUS  
(17) Schoenenberger, C; Electrochim Acta 1995, V40, P2281  
CAPLUS

(18) Watanabe, M; Polym J 1986, V11, P909  
 (19) Williams, M; J Am Chem Soc 1955, V77, P3701 CAPLUS  
 (20) Wright, P; Br Polym J 1975, V7, P319 CAPLUS

L2 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 439659-56-0 REGISTRY  
 ED Entered STN: 21 Jul 2002  
 CN Oxetane, 3,3'-(2,5,8,11-tetraoxadodecane-1,12-diyl)bis[3-ethyl-, polymer  
 with 3-(2,5,8,11,14,17,20,23,26,29-decaoxatriacont-1-yl)-3-ethyloxetane  
 (9CI) (CA INDEX NAME)  
 MF (C25 H50 O11 . C18 H34 O6)x  
 CI PMS  
 PCT Polyether, Polyether formed  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAplus document type: Journal  
 RLD.NP Roles for non-specific derivatives from non-patents: PREP  
 (Preparation); PRP (Properties)

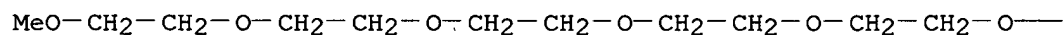
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EA	ES	SZ	RF	RID	Count
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					1 2 in CM
					2

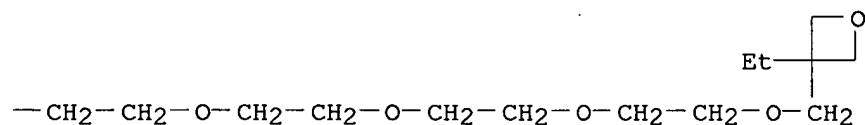
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CRN 439659-52-6  
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PAGE 1-A

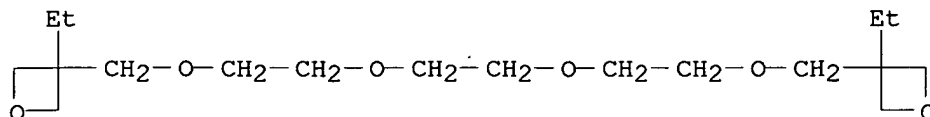


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CM 2

CRN 369404-92-2  
 CMF C18 H34 O6



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

ACCESSION NUMBER: 137:63573 CA  
 TITLE: Novel polymer electrolytes based on mono- and bis-oxetane monomers with oligo(ethylene oxide) units  
 AUTHOR(S): Miwa, Yoshiyuki; Tsutsumi, Hiromori; Oishi, Tsutomu  
 CORPORATE SOURCE: Ube Laboratory, Ube Ind. Ltd., Ube, Yamaguchi, 755-8633, Japan  
 SOURCE: Electrochemistry (Tokyo, Japan) (2002), 70(4), 264-269  
 CODEN: EECTFA; ISSN: 1344-3542  
 PUBLISHER: Electrochemical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)  
 Section cross-reference(s): 36, 76

#### ABSTRACT:

Polymer electrolytes were prepared by cationic ring-opening polymerization of bis-oxetane (R-O-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>m</sub>-R, R = 3-ethyl-3-methylene oxetane, DDOE (m = 2), TrDOE (m = 3), TeDOE (m = 4)) and mono-oxetane (R-O-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>n</sub>-CH<sub>3</sub>, TrMOE (n = 3), NoMOE (n = 9), DoMOE (n = 12)) with lithium salt catalyst. The polyethers were characterized by differential scanning calorimetry (DSC) and alternating impedance spectroscopy. The poly(oxetane)-based electrolytes have crosslinked networks with oligo(ethylene oxide) and 2-ethyltrimethylene oxide main chains and methoxy-oligo(ethylene oxide) side chains. The polymer electrolytes prepared with LiBF<sub>4</sub> have high ionic conductivity, compared to that of polymers prepared with LiPF<sub>6</sub> or LiN(C<sub>2</sub>F<sub>5</sub>SO<sub>2</sub>)<sub>2</sub>. The conductivity of the poly(oxetane)-LiBF<sub>4</sub> complexes depended on the mono-oxetane content and the length of oligo(ethylene oxide) in the mono- and bis-oxetanes. The oligo(ethylene oxide) side chains in the complexes act as efficient plasticizing agents, particularly NoMOE and DoMOE. Maximum conductivity of the polymer electrolytes with LiBF<sub>4</sub> ([Li]/[O] = 0.045) was 9.1 x 10<sup>-6</sup> (TrMOE/DDOE mole ratio = 3.0) and 1.0 x 10<sup>-4</sup> S-cm<sup>-1</sup> (NoMOE/DDOE = 1.72 and DoMOE/DDOE = 1.29).

SUPPL. TERM: oxetane ring opening polymn polyether prepn lithium salt catalyst; electrolyte polyether oxetane lithium tetrafluoroborate complex cond; ionic cond electrolyte polyether oxetane lithium salt; oligoethylene oxide side chain oxetane polyether glass transition temp  
 INDEX TERM: Polymerization  
 Polymerization catalysts  
 (cationic, ring-opening; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)  
 INDEX TERM: Polyoxyalkylenes, preparation  
 ROLE: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (oxetane-derived; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization)

with lithium salts as catalysts and counterion source)

INDEX TERM: Glass transition temperature  
Ionic conductivity  
Polymer electrolytes  
(preparation and ionic conductivity vs. temperature of  
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INDEX TERM: 383364-44-1P, (3-Ethyl-3-oxetanyl)-2,5,8,11-tetraoxadodecane  
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ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
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INDEX TERM: 14283-07-9 21324-40-3, Lithium hexafluorophosphate (LiPF<sub>6</sub>)  
132843-44-8, Lithium bis(pentafluoroethylsulfonyl)imide  
ROLE: CAT (Catalyst use); PRP (Properties); USES (Uses)  
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L2 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 439659-55-9 REGISTRY  
 ED Entered STN: 21 Jul 2002  
 CN Oxetane, 3,3'-[oxybis(2,1-ethanediylloxymethylene)]bis[3-ethyl-, polymer with 3-ethyl-3-(2,5,8,11,14,17,20,23,26,29,32,35,38-tridecaoxanonatriacont-1-yl)oxetane (9CI) (CA INDEX NAME)  
 MF (C31 H62 O14 . C16 H30 O5)x  
 CI PMS  
 PCT Polyether, Polyether formed  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAplus document type: Journal  
 RLD.NP Roles for non-specific derivatives from non-patents: PREP  
 (Preparation); PRP (Properties)

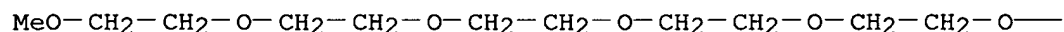
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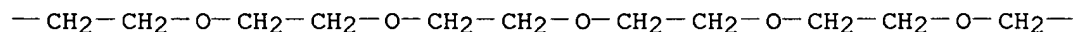
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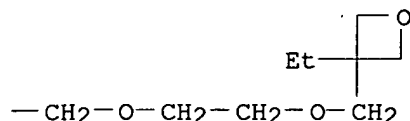
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PAGE 1-B

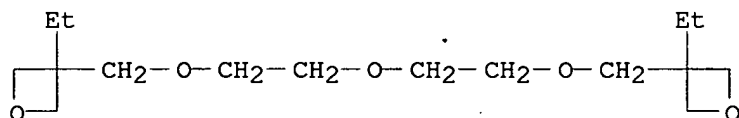




CM 2

CRN 303109-63-9

CMF C16 H30 O5



- 1 REFERENCES IN FILE CA (1907 TO DATE)  
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 AUTHOR(S): Miwa, Yoshiyuki; Tsutsumi, Hiromori; Oishi, Tsutomu  
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SUPPL. TERM: oxetane ring opening polymn polyether prepn lithium salt catalyst; electrolyte polyether oxetane lithium



tetrafluoroborate complex cond; ionic cond electrolyte  
 polyether oxetane lithium salt; oligoethylene oxide side  
 chain oxetane polyether glass transition temp  
 INDEX TERM: Polymerization  
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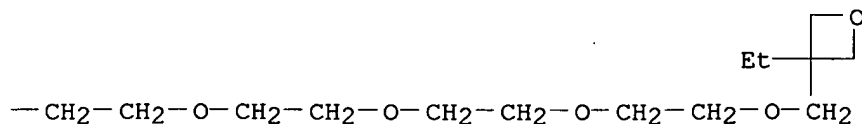
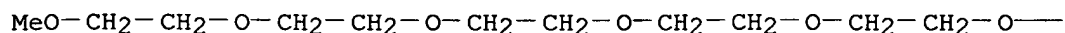
L2 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 439659-54-8 REGISTRY  
ED Entered STN: 21 Jul 2002  
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with 3-(2,5,8,11,14,17,20,23,26,29-decaoxatriacont-1-yl)-3-ethyloxetane  
(9CI) (CA INDEX NAME)  
MF (C25 H50 O11 . C16 H30 O5)x  
CI PMS  
PCT Polyether, Polyether formed  
SR CA  
LC STN Files: CA, CAPLUS  
DT.CA Caplus document type: Journal  
RLD.NP Roles for non-specific derivatives from non-patents: PREP  
(Preparation); PRP (Properties)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
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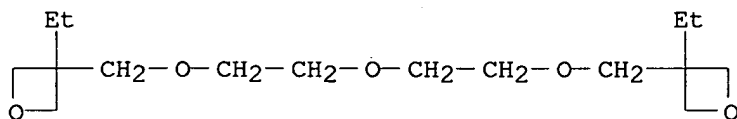
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CM 2

CRN 303109-63-9

CMF C16 H30 O5



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L2 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN

RN 439659-53-7 REGISTRY

ED Entered STN: 21 Jul 2002

CN Oxetane, 3-ethyl-3-(2,5,8,11,14,17,20,23,26,29,32,35,38-  
tridecaoxanonatriacont-1-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN (3-Ethyl-3-oxetanyl)-2,5,8,11,14,17,20,23,26,29,32,35,38-  
tridecaoxanonatriacontane

FS 3D CONCORD

MF C31 H62 O14

CI COM

SR CA

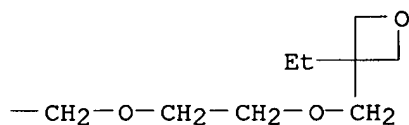
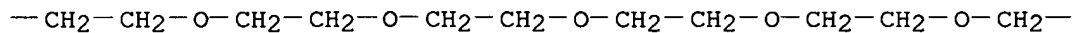
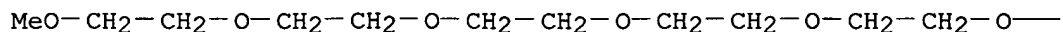
LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C30	OC3	4	C30	4.214.1	1



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1	pH 10	(1) ACD
Boiling Point (BP)	644.9+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	91.67+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	227.7+/-54.0 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	39		(1) ACD
H acceptors (HAC)	14		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	1	pH 10	(1) ACD
logD (LOGD)	-3.74	pH 1	(1) ACD
logD (LOGD)	-3.74	pH 4	(1) ACD
logD (LOGD)	-3.74	pH 7	(1) ACD
logD (LOGD)	-3.74	pH 8	(1) ACD
logD (LOGD)	-3.74	pH 10	(1) ACD
logP (LOGP)	-3.743+/-0.867		(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 10	(1) ACD

Molecular Weight (MW) | 658.82 | | (1) ACD  
Vapor Pressure (VP) | 8.22E-16 Torr | 25.0 deg C | (1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

ACCESSION NUMBER: 137:63573 CA  
TITLE: Novel polymer electrolytes based on mono- and  
bis-oxetane monomers with oligo(ethylene oxide) units  
AUTHOR(S): Miwa, Yoshiyuki; Tsutsumi, Hiromori; Oishi, Tsutomu  
CORPORATE SOURCE: Ube Laboratory, Ube Ind. Ltd., Ube, Yamaguchi,  
755-8633, Japan  
SOURCE: Electrochemistry (Tokyo, Japan) (2002), 70(4), 264-269  
CODEN: EECTFA; ISSN: 1344-3542  
PUBLISHER: Electrochemical Society of Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 36, 76

#### ABSTRACT:

Polymer electrolytes were prepared by cationic ring-opening polymerization of bis-oxetane (R-O-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>m</sub>-R, R = 3-ethyl-3-methylene oxetane, DDOE (m = 2), TrDOE (m = 3), TeDOE (m = 4)) and mono-oxetane (R-O-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>n</sub>-CH<sub>3</sub>, TrMOE (n = 3), NoMOE (n = 9), DoMOE (n = 12)) with lithium salt catalyst. The polyethers were characterized by differential scanning calorimetry (DSC) and alternating impedance spectroscopy. The poly(oxetane)-based electrolytes have crosslinked networks with oligo(ethylene oxide) and 2-ethyltrimethylene oxide main chains and methoxy-oligo(ethylene oxide) side chains. The polymer electrolytes prepared with LiBF<sub>4</sub> have high ionic conductivity, compared to that of polymers prepared with LiPF<sub>6</sub> or LiN(C<sub>2</sub>F<sub>5</sub>SO<sub>2</sub>)<sub>2</sub>. The conductivity of the poly(oxetane)-LiBF<sub>4</sub> complexes depended on the mono-oxetane content and the length of oligo(ethylene oxide) in the mono- and bis-oxetanes. The oligo(ethylene oxide) side chains in the complexes act as efficient plasticizing agents, particularly NoMOE and DoMOE. Maximum conductivity of the polymer electrolytes with LiBF<sub>4</sub> ([Li]/[O] = 0.045) was 9.1 x 10<sup>-6</sup> (TrMOE/DDOE mole ratio = 3.0) and 1.0 x 10<sup>-4</sup> S-cm<sup>-1</sup> (NoMOE/DDOE = 1.72 and DoMOE/DDOE = 1.29).

SUPPL. TERM: oxetane ring opening polymn polyether prepn lithium salt  
catalyst; electrolyte polyether oxetane lithium  
tetrafluoroborate complex cond; ionic cond electrolyte  
polyether oxetane lithium salt; oligoethylene oxide side  
chain oxetane polyether glass transition temp  
INDEX TERM: Polymerization  
Polymerization catalysts  
(cationic, ring-opening; preparation and ionic conductivity  
vs. temperature  
of oxetane-polyether electrolytes by ring opening  
polymerization  
with lithium salts as catalysts and counterion source)  
INDEX TERM: Polyoxyalkylenes, preparation  
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(oxetane-derived; preparation and ionic conductivity vs.  
temperature of

oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: Glass transition temperature  
Ionic conductivity  
Polymer electrolytes  
(preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: 383364-44-1P, (3-Ethyl-3-oxetanyl)-2,5,8,11-tetraoxadodecane  
439659-52-6P, (3-Ethyl-3-oxetanyl)-2,5,8,11,14,17,20,23,26,29-decaoxatriacontane  
439659-53-7P, (3-Ethyl-3-oxetanyl)-2,5,8,11,14,17,20,23,26,29,32,35,38-tridecaoxanonatriacontane  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(monomer; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: 14283-07-9 21324-40-3, Lithium hexafluorophosphate (LiPF<sub>6</sub>)  
132843-44-8, Lithium bis(pentafluoroethylsulfonyl)imide  
ROLE: CAT (Catalyst use); PRP (Properties); USES (Uses)  
(polymerization catalyst and electrolyte; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: 7439-93-2DP, Lithium, complexes with poly(oxetane-ether)s  
383364-45-2DP, lithium complexes 439659-54-8DP, lithium complexes  
439659-55-9DP, lithium complexes  
439659-56-0DP, lithium complexes 439659-57-1DP, lithium complexes  
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: 112-35-6, Triethylene glycol monomethyl ether 3047-32-3, 3-Ethyl-3-hydroxymethyloxetane 5702-16-9, Dodecaethylene glycol monomethyl ether 6048-68-6, Nonaethylene glycol monomethyl ether  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Abraham, K; Electrochim Acta 1993, V38, P1233 CAPLUS  
(2) Berthier, C; Solid State Ionics 1983, V11, P91 CAPLUS  
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## CAPLUS

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 (13) Papke, B; J Electrochem Soc 1982, V129, P1434 CAPLUS  
 (14) Papke, B; J Electrochem Soc 1982, V129, P1694 CAPLUS  
 (15) Pattison, D; J Am Chem Soc 1957, V79, P3455 CAPLUS  
 (16) Ratner, M; Chem Rev 1988, V88, P109 CAPLUS  
 (17) Schoenenberger, C; Electrochim Acta 1995, V40, P2281

## CAPLUS

- (18) Watanabe, M; Polym J 1986, V11, P909  
 (19) Williams, M; J Am Chem Soc 1955, V77, P3701 CAPLUS  
 (20) Wright, P; Br Polym J 1975, V7, P319 CAPLUS

L2 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2005 ACS on STN

RN 439659-52-6 REGISTRY

ED Entered STN: 21 Jul 2002

CN Oxetane, 3-(2,5,8,11,14,17,20,23,26,29-decaoxatriacont-1-yl)-3-ethyl-  
 (9CI) (CA INDEX NAME)

## OTHER NAMES:

CN (3-Ethyl-3-oxetanyl)-2,5,8,11,14,17,20,23,26,29-decaoxatriacontane

FS 3D CONCORD

MF C25 H50 O11

CI COM

SR CA

LC STN Files: CA, CAPLUS

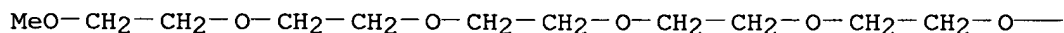
DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

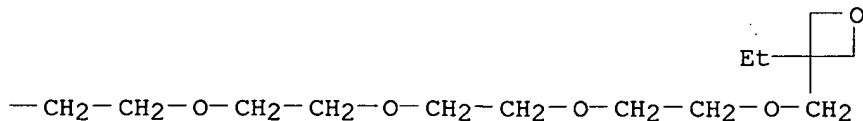
## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
=====	+	=====	+	=====	+
C3O	OC3	4	C3O	4.214.1	1

PAGE 1-A



PAGE 1-B



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1	pH 10	(1) ACD
Boiling Point (BP)	553.7+/-45.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	80.34+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	204.1+/-51.5 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	30		(1) ACD
H acceptors (HAC)	11		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	1	pH 10	(1) ACD
logD (LOGD)	-2.67	pH 1	(1) ACD
logD (LOGD)	-2.67	pH 4	(1) ACD
logD (LOGD)	-2.67	pH 7	(1) ACD
logD (LOGD)	-2.67	pH 8	(1) ACD
logD (LOGD)	-2.67	pH 10	(1) ACD
logP (LOGP)	-2.669+/-0.800		(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	526.66		(1) ACD
Vapor Pressure (VP)	9.82E-12 Torr	25.0 deg C	(1) ACD

(1). Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

ACCESSION NUMBER: 137:63573 CA  
TITLE: Novel polymer electrolytes based on mono- and bis-oxetane monomers with oligo(ethylene oxide) units  
AUTHOR(S): Miwa, Yoshiyuki; Tsutsumi, Hiromori; Oishi, Tsutomu  
CORPORATE SOURCE: Ube Laboratory, Ube Ind. Ltd., Ube, Yamaguchi, 755-8633, Japan  
SOURCE: Electrochemistry (Tokyo, Japan) (2002), 70(4), 264-269  
CODEN: EECTFA; ISSN: 1344-3542  
PUBLISHER: Electrochemical Society of Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
CLASSIFICATION: 35-7 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 36, 76

#### ABSTRACT:

Polymer electrolytes were prepared by cationic ring-opening polymerization of bis-oxetane (R-O-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>m</sub>-R, R = 3-ethyl-3-methylene oxetane, DDOE (m = 2), TrDOE (m = 3), TeDOE (m = 4)) and mono-oxetane (R-O-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>n</sub>-CH<sub>3</sub>, TrMOE (n = 3), NoMOE (n = 9), DoMOE (n = 12)) with lithium salt catalyst. The polyethers were characterized by differential scanning calorimetry (DSC) and alternating impedance spectroscopy. The poly(oxetane)-based electrolytes have crosslinked

networks with oligo(ethylene oxide) and 2-ethyltrimethylene oxide main chains and methoxy-oligo(ethylene oxide) side chains. The polymer electrolytes prepared with LiBF<sub>4</sub> have high ionic conductivity, compared to that of polymers prepared with LiPF<sub>6</sub> or LiN(C<sub>2</sub>F<sub>5</sub>SO<sub>2</sub>)<sub>2</sub>. The conductivity of the poly(oxetane)-LiBF<sub>4</sub> complexes depended on the mono-oxetane content and the length of oligo(ethylene oxide) in the mono- and bis-oxetanes. The oligo(ethylene oxide) side chains in the complexes act as efficient plasticizing agents, particularly NoMOE and DoMOE. Maximum conductivity of the polymer electrolytes with LiBF<sub>4</sub> ([Li]/[O] = 0.045) was 9.1 x 10<sup>-6</sup> (TrMOE/DDOE mole ratio = 3.0) and 1.0 x 10<sup>-4</sup> S-cm<sup>-1</sup> (NoMOE/DDOE = 1.72 and DoMOE/DDOE = 1.29).

SUPPL. TERM: oxetane ring opening polymn polyether prepn lithium salt catalyst; electrolyte polyether oxetane lithium tetrafluoroborate complex cond; ionic cond electrolyte polyether oxetane lithium salt; oligoethylene oxide side chain oxetane polyether glass transition temp

INDEX TERM: Polymerization  
Polymerization catalysts  
(cationic, ring-opening; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: Polyoxyalkylenes, preparation  
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(oxetane-derived; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: Glass transition temperature  
Ionic conductivity  
Polymer electrolytes  
(preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: 383364-44-1P, (3-Ethyl-3-oxetanyl)-2,5,8,11-tetraoxadodecane  
439659-52-6P, (3-Ethyl-3-oxetanyl)-2,5,8,11,14,17,20,23,26,29-decaoxatriacontane  
439659-53-7P, (3-Ethyl-3-oxetanyl)-2,5,8,11,14,17,20,23,26,29,32,35,38-tridecaoxanonatriacontane  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(monomer; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: 14283-07-9 21324-40-3, Lithium hexafluorophosphate (LiPF<sub>6</sub>)  
132843-44-8, Lithium bis(pentafluoroethylsulfonyl)imide  
ROLE: CAT (Catalyst use); PRP (Properties); USES (Uses)  
(polymerization catalyst and electrolyte; preparation and ionic conductivity vs. temperature of oxetane-polyether electrolytes by ring opening polymerization with lithium salts as catalysts and counterion source)

INDEX TERM: 7439-93-2DP, Lithium, complexes with poly(oxetane-ether)s  
383364-45-2DP, lithium complexes 439659-54-8DP, lithium complexes 439659-55-9DP, lithium complexes 439659-56-0DP, lithium complexes 439659-57-1DP, lithium

complexes  
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(preparation and ionic conductivity vs. temperature of

oxetane-polyether

electrolytes by ring opening polymerization with lithium salts  
as catalysts and counterion source)

INDEX TERM: 112-35-6, Triethylene glycol monomethyl ether 3047-32-3,  
3-Ethyl-3-hydroxymethyloxetane 5702-16-9, Dodecaethylene  
glycol monomethyl ether 6048-68-6, Nonaethylene glycol  
monomethyl ether

ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(preparation and ionic conductivity vs. temperature of

oxetane-polyether

electrolytes by ring opening polymerization with lithium salts  
as catalysts and counterion source)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
RECORD.

REFERENCE(S): (1) Abraham, K; Electrochim Acta 1993, V38, P1233 CAPLUS  
(2) Berthier, C; Solid State Ionics 1983, V11, P91 CAPLUS  
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(10) Miwa, Y; Polym J 2001, V33, P568 CAPLUS  
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(15) Pattison, D; J Am Chem Soc 1957, V79, P3455 CAPLUS  
(16) Ratner, M; Chem Rev 1988, V88, P109 CAPLUS  
(17) Schoenenberger, C; Electrochim Acta 1995, V40, P2281  
CAPLUS  
(18) Watanabe, M; Polym J 1986, V11, P909  
(19) Williams, M; J Am Chem Soc 1955, V77, P3701 CAPLUS  
(20) Wright, P; Br Polym J 1975, V7, P319 CAPLUS

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